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Regulatory Water Quality Monitoring Networks

Statistical and Economic Considerations

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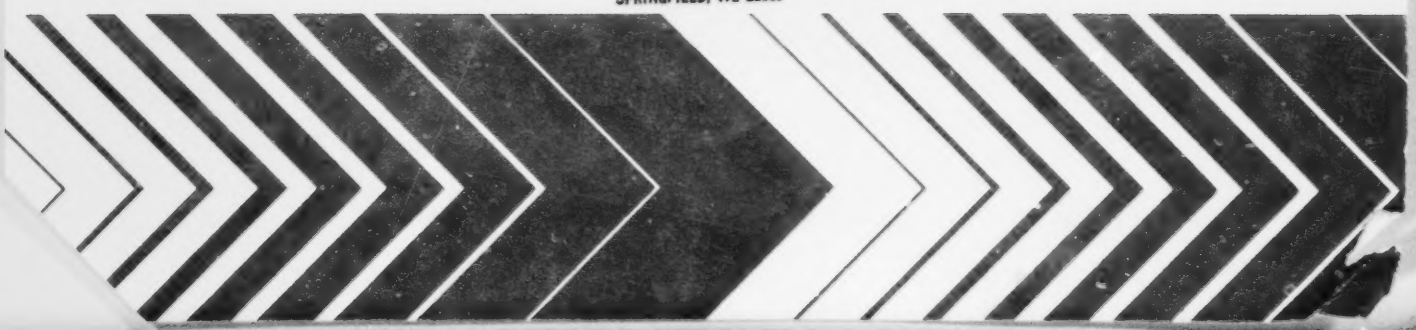

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16. ABSTRACT

The purpose of this study is to examine and quantify the statistical trade-offs associated with using various levels of statistical sophistication in network design and to formulate a procedure for accounting for economic constraints in design process. Sampling frequency is the major aspect of network design considered in the study; consequently, the results of the study are directed toward their use by regulatory agencies for the evaluation and upgrading of existing networks.

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REGULATORY WATER QUALITY MONITORING NETWORKS--
STATISTICAL AND ECONOMIC CONSIDERATIONS

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FOREWORD

Protection of the environment requires effective regulatory actions that are based on sound technical and scientific information. This information must include the quantitative description and linking of pollutant sources, transport mechanisms, interactions, and resulting effects on man and his environment. Because of the complexities involved, assessment of specific pollutants in the environment requires a total systems approach that transcends the media of air, water, and land. The Environmental Monitoring and Support Laboratory-Las Vegas contributes to the formation and enhancement of a sound monitoring data base for exposure assessment through programs designed to:

- develop and optimize systems and strategies for monitoring pollutants and their impact on the environment
- demonstrate new monitoring systems and technologies by applying them to fulfill special monitoring needs of the Agency's operating programs.

This report covers a procedure for evaluating sampling frequencies of established water quality monitoring networks. This report is intended to assist monitoring systems managers to more efficiently distribute resources between sampling sites and laboratory facilities in an effort to achieve better data at a lower cost. For further information contact the Monitoring Systems Research and Development Division at this Laboratory.

George B. Morgan
Director
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Las Vegas

SUMMARY

During the past eight years, a number of procedures have been proposed for designing fixed-station water quality monitoring networks for regulatory water quality management purposes. Each new procedure is based upon a specific, and increasingly higher, level of statistical analysis and may or may not consider the economics of monitoring. As the statistics applied to the monitoring network design have become more and more sophisticated, practical use of the design procedures has become more confusing, especially in light of the economic constraints under which all regulatory agencies operate.

The purpose of this study is to examine and quantify the statistical trade-offs associated with using various levels of statistical sophistication in network design and to formulate a procedure for accounting for economic constraints in the design process. Sampling frequency is the major aspect of network design considered in the study; consequently, the results of the study are directed toward use by regulatory agencies for the evaluation and upgrading of existing networks.

Network design can be based on a number of different objectives; however, it is becoming increasingly clear that the estimate of trends is the major goal of fixed-station networks (mainly because of the low sampling frequencies used). Consequently, the network objective selected for this statistical comparison study was that of estimating annual geometric means of water quality variables within known or projected confidence intervals. The sampling frequency that achieves the desired confidence interval is then designated the sampling frequency for the network.

Three levels of statistical sophistication were analyzed by computing the confidence intervals about the geometric mean using:

1. A variance that accounted for seasonal variation and serial correlation.

2. A variance that accounted for only seasonal variation.

3. A variance computed directly from the original data (i.e., no accounting for either seasonal variation or serial correlation).

In order to compute the first two variances with confidence and to consider network design, one must have a rather extensive water quality record (e.g., frequent sampling over a long period of time for a range of water quality variables and from a network of stations). Such records are rare; however, an Illinois record met all of the criteria except the long

period of time. It was a one-year record with daily sampling at nine stations covering 26 variables. The data record does permit a comparison of the statistical levels in network design.

In order to compute the second variance, seasonal variation was assumed to be deterministic and able to be predicted by estimating the coefficients A and C of the equation:

$$y_t = A (\cos wt + C)$$

where y_t = deterministic component at time t

w = 360 degrees/number of samples per year

The deterministic seasonal variation was then subtracted from the original data and the variance computed.

The data from the above calculations were analyzed next to determine the correlation structures. This was accomplished by fitting the coefficients, ϕ_1, ϕ_2, and θ_1, of the autoregressive, moving-average model:

$$Z_t = \phi_1 Z_{t-1} + \phi_2 Z_{t-2} + a_t - \theta_1 a_{t-1}$$

where Z_t = value of time series at time t

a_t = random noise at time t

for each water quality variable. The theoretical autocorrelation functions were then calculated based on the fitted models. The first variance could then be determined.

Confidence intervals were computed for each station and for each variable. The confidence intervals using the first variance were assumed to be correct since they included the most sophisticated analysis. Confidence intervals with variances 2 and 3 were then compared.

Results indicate that, within a sampling frequency range of approximately 12 samples per year to 34 samples per year, there is only an 8 to 10 percent error in confidence intervals about the means between the simplest and most sophisticated design approaches. In this range the effects of seasonal variation and serial correlation tend to cancel each other out, so either both must be considered or both ignored. Since this is the range within which many regulatory agencies operate their networks, it appears that using basic statistics in network design is sufficient, especially in light of the limited data records available to support more sophisticated network design statistics. It should be pointed out that the above range of frequencies is an average over five water quality variables--individual variables may act quite differently from the average.

A dynamic programming code was formulated to assign sampling frequencies throughout a network with the goal of optimizing a statistical objective function subject to an economic constraint. The objective function is the sum (over several variables and all stations) of the normalized positive deviation of the predicted confidence interval widths from preselected design confidence interval widths. The code was designed to account for the effects of deterministic seasonal variation and serial correlation by incorporating the results of the time-series analysis described above. The economic constraint ensures that the annual operating costs of travel and laboratory analysis will not exceed the allowable budget.

Within the economic framework used in this study, which deals strictly with the operating costs of a monitoring system at a fixed scale of operation, the dynamic programming solution is relatively insensitive to variation in the laboratory analysis and travel costs. The solution is more stongly influenced by the water quality variables included in the design and by the selection of design confidence interval widths.

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LIST OF ABBREVIATIONS AND SYMBOLS

ABBREVIATIONS

ARMA	--	autoregressive, moving-average
mg/ℓ	--	milligrams per liter
SS	--	suspended solids
TDS	--	total dissolved solids
TOC	--	total organic carbon

SYMBOLS

A	--	amplitude of deterministic annual water quality cycle
a_t	--	white-noise component or shock at time t in ARMA process
C	--	phase angle of deterministic annual water quality cycle
C_i	--	annual operating cost of sampling for station i
$\text{cov}(x,y)$	--	covariance of x and y
C_T	--	total annual operating budget for network
$f_i(S_i, u_i)$	--	return function in dynamic programming
$f_i^*(S_i)$	--	optimal return function in dynamic programming
I_{ij}	--	information content for station i, constituent j
I_j^D	--	design information content for constituent j
$K_{\alpha/2}$	--	standard normal deviate for a probability of $\alpha/2$
m	--	slope of deterministic linear trend in water quality
M	--	number of water quality constituents included in design
N	--	number of stations in network

NC_3	--	nitrate
Q	--	test statistic used in ARMA model evaluation
R	--	one-half the confidence interval width
$r_k(a)$	--	estimate of lag-k autocorrelation of residuals in ARMA model evaluation
S_i	--	state variable for stage i in dynamic programming (budget remaining)
T	--	period of cycle (in this report, one year)
u_i	--	decision variable for stage i in dynamic programming (number of samples collected per year at station i)
$u_i^*(S_i)$	--	optimal decision function in dynamic programming
$var(X)$	--	variance of X
$\bar{X}$	--	sample mean of X
X_{ij}	--	confidence interval width for constituent j at station i
X_j^D	--	design confidence interval width for constituent j
X_t	--	value of water quality time series at time t
y_t	--	value of deterministic annual cycle in water quality at time t
Z_t	--	value of water quality time series at time t after seasonal variation is removed
α	--	statistical significance level
χ^2_n	--	$(1-\alpha)$th quantile of chi-square distribution with n degrees of freedom
θ_q	--	qth moving average coefficent of an ARMA process
μ	--	population mean (of a water quality variable)
μ'	--	population geometric mean (of a water quality variable)
$\rho(n)$ or ρ_n	--	lag-n autocorrelation coefficient
σ^2	--	population variance of water quality random variable

σ_a^2 -- white-noise variance of a water quality time series

σ_z^2 -- variance of a water quality time series with seasonal variation removed

σ_{ij}^2 -- variance of water quality constituent j at station i

ϕ_p -- pth autoregressive coefficient of an ARMA process

SECTION 1

INTRODUCTION

In the area of water pollution, Federal law contains well defined procedures for planning and implementing pollution control measures by local, State, and Federal government agencies. Throughout the pertinent body of legislation (PL 89-234, PL 92-500, and PL 95-217, the Clean Water Act) and plans that have arisen from implementation of the law, there exists an almost universal recognition of the need for regulatory water quality monitoring in support of pollution control activities. Regulatory monitoring is defined here as routine, fixed-station monitoring performed by a water quality management agency to support its regulatory functions, such as discharge, permit issuance and renewal.

Unfortunately, neither the nature and scope nor the precise statistical objectives of such monitoring programs have been spelled out. Thus regulatory monitoring systems have often been put into service in response to demands for immediate action and without the careful thinking beforehand that is necessary to ensure success.

Researchers in both government and academic institutions have declared that much of this careful thinking in relation to water quality data collection should occur through consideration of statistical concepts. As a result, the application of statistical methods to the design of surface water monitoring systems has received much attention in recent years, and considerable research has been conducted in an attempt to develop statistically sound design procedures. One might hope that all of this work has led to a fairly widespread acceptance of some basic principles that could be applied in practical situations. Unfortunately this is not the case. Rather one is confronted with many diverse opinions as to what sort of statistical approach and what level of statistical sophistication to apply to the design of regulatory water quality monitoring networks. Several design procedures have been proposed, each based on one opinion or another, but none seem to have made it into the hands of water quality management agencies who are required by law to collect water quality data and who, consequently, collect a significant percentage of all the water quality data in the United States.

Thus the monitoring efforts of many, if not most, management agencies have been criticized, and the value of information they collect has been questioned.

A second major concern in the design of monitoring networks is that of achieving cost effectiveness in operation. Although the final judgment of

whether or not the dollars devoted to monitoring are being well spent rests on a difficult and subjective evaluation of the worth of data records, the problem of improving statistical and economic efficiency in existing monitoring programs is more straightforward. The above statements regarding the inadequacy of current water quality monitoring practices are explained more fully in a report by the National Academy of Sciences (1977).

This research effort was undertaken in an attempt to refine currently available scientific tools and to investigate their potential for application to these two problems--the statistics and economics of water quality sampling. The results of the research are directed toward use by regulatory water quality management agencies for the twofold purpose of evaluating and upgrading their regulatory water quality monitoring programs.

The project involves the analysis of historic water quality records for the purpose of reassigning sampling frequencies within a network. The level of statistical sophistication employed is somewhat beyond the current capabilities of most water quality management agencies. The practical realities of applying this approach are then weighed against the consequences of using only elementary statistics in sampling frequency design.

Finally, a mathematical programming procedure is developed that can make use of statistical information (at any level of sophistication) to assign sampling frequencies within a network while operating at a fixed budgetary level.

OBJECTIVES

The overall objective of this research is to develop procedures for evaluating and upgrading regulatory water quality monitoring networks in terms of their ability to achieve desirable confidence interval widths about sample geometric means for selected measured variables. This overall objective is accomplished via the following detailed objectives:

1. To identify a method for calculating the confidence interval width about the sample mean or geometric mean of water quality variables (concentrations of constituents) for given sampling frequencies when the sample observations form a correlated time series.

2. To compare the results of computing confidence interval widths using the same method as above with those obtained using simpler statistical approaches.

3. To incorporate both statistical and economic information into sampling frequency design by formulating and solving a mathematical programming problem. The solution should minimize the overall difference between design confidence interval widths and predicted confidence interval widths throughout a network while operating at a fixed budgetary level.

The first objective is accomplished through analysis of historic water quality records. The time series of observations is assumed to consist of three components: a linear trend, an annual cycle, and a correlated noise

component. Each of these components is modeled, and the effects of each are accounted for in the computation of confidence intervals.

The second objective is accomplished by incorporating the results of the first objective into a dynamic programming algorithm along with a provision for computing the operating cost of sampling at individual stations. The algorithm assigns sampling frequencies to each station in a network in order to achieve optimum size and uniformity of confidence interval widths about sample means or geometric means when considering several water quality constituents simultaneously. A fixed annual operating budget is imposed as a constraint.

Several basic assumptions are necessary. The assumptions that delineate the scope of the research are as follows:

1. An adequate historic data record is available for each water quality constituent and each station under consideration.

2. Future grab samples will be equally spaced in time.

3. Sampling frequencies for all water quality constituents at a given station are identical--i.e., each sample will be analyzed for all constituents.

4. The selection of constituents to be measured is assumed to have been performed beforehand.

5. Water quality observations from the data records used are assumed to be representative in both time and space of conditions that actually existed at the station.

6. The variance of the estimates of annual means of the water quality variables as a result of poor sampling procedure or laboratory error is ignored.

7. The variance of the estimates of parameters in deterministic and stochastic models used in computing confidence interval widths about the annual means are ignored as well.

ORGANIZATION OF THE REPORT

The remainder of this report is organized in the following manner. Section 2 contains a review of literature covering the current state of water quality monitoring, statistical tools appropriate for designing stream quality monitoring systems, and several approaches to design that have been suggested in the past. Section 3 develops in detail those statistical methods (including time series analysis) that are necessary for applying the confidence interval approach to the assignment of sampling frequencies while considering seasonal variation and serial correlation in water quality. The methods are illustrated by application to data records from three areas: (1) the Red River, Manitoba; (2) Grand River, Michigan; and (3) a nine-station network in the State of Illinois. In Section 4 the dynamic programming algorithm is

developed and applied to the Illinois network. A sensitivity analysis explores the effect of variation of the major input variables. Sections 5 and 6 conclude the report with a discussion of the practical implications of the research, a brief summary statement, and suggestions for further research.

SECTION 2

CONCLUSIONS

1. The effect of serial correlation on confidence interval widths about annual means is important at high sampling frequencies and lessens as the sampling frequency decreases. The point at which the effect of serial correlation becomes insignificant varies among water quality constituents and locations, depending on the correlation structure of the individual time series. Typically, however, this point will occur at a sampling interval of three to five weeks.

2. The deterministic annual cycle significantly affects computed confidence interval widths over the entire range of sampling frequencies under consideration--daily to bimonthly. Experimental results indicate that failure to account for this seasonal variation can result in computation of confidence interval widths that are 20 percent to 50 percent larger than those that actually apply within this range of sampling frequencies.

3. For the water quality time series studied and for a certain range of sampling intervals, typically two to four weeks, the effects of serial correlation in computing confidence interval widths is roughly offset by the effects of seasonal variation. Therefore within this region, both of the above factors should be considered in computing confidence interval widths, or neither should be considered.

4. The water quality records studied in this research indicate that the most likely candidate models of the ARMA type to be evaluated for water quality time series are AR(1), AR(2), and ARMA (1,1).

5. Computed confidence interval widths about annual means are highly sensitive to the value of the lag-one autocorrelation coefficient of the time series in question. Estimated values of ρ_1 encountered in this research range from approximately 0.5 to 0.9.

6. The dynamic programming code presented in this report provides a fairly simple, efficient means of assigning sampling frequencies throughout a network. The code is particularly useful when it is desired to include the effect of serial correlation in the computation of confidence interval widths and when the selection of sampling frequencies is limited to a few allowable values.

7. Within the economic framework used in this study, which deals strictly with the operating costs of a monitoring system at a fixed scale of operation, the dynamic programming solution is relatively insensitive to variation in the laboratory analysis and travel costs. The solution is more strongly influenced, however, by the water quality constituents included in the design and by the selection of design confidence interval widths.

SECTION 3

RECOMMENDATIONS

Two groups of recommendations are made. The first group deals with application of the current research, and the second group deals with suggestions for future research.

RECOMMENDATIONS FOR APPLICATION

1. The effect of serial correlation on the widths of confidence intervals about annual means or geometric means of quality constituents should be considered by water quality management agencies for sampling intervals of one month or less. These effects are important in both the design of regulatory monitoring networks and the analysis of data subsequently collected for management decisions.

2. The serial correlation effects should be quantified via the time series analysis procedures described herein if sufficient data records are available. An assumed AR(1) correlation structure with a regionalized or estimated value of the lag-one autocorrelation coefficient is the suggested alternative.

3. In analyzing water quality records, a deterministic annual cycle should be computed and removed from the observations prior to the determination of confidence interval widths whenever possible. A fairly long record is needed for this purpose, but equally spaced observations are not required.

4. In future water quality monitoring systems, samples should be collected equally spaced in time to facilitate time series analysis and trend detection.

5. Sampling frequencies should be allocated among various stations of a regulatory network using some rational statistical basis. The dynamic programming code presented here is suggested with linear programming and a stratified sampling approach as alternatives. The mathematical programming approaches are preferable because they allow the incorporation of economics into the analysis.

6. Management agencies should attempt to quantify as accurately as possible the direct costs of travel and laboratory analysis that they experience in sample collection and processing. The economic viewpoint adopted here assumes that these costs are accurately known in order to establish the

annual operating budget. Thus these cost figures are critical in the economic analysis even though the sensitivity analysis showed the example dynamic programming solution to be relatively insensitive to changes in them.

7. The eventual uses of water quality data in management decisions should be considered in the design of regulatory monitoring networks, particularly with respect to the selection of water quality constituents to be included in the design.

SUGGESTIONS FOR FUTURE RESEARCH

1. Daily water quality data for several constituents should be collected at several locations in various sections of the United States over a long period of time.

2. Such daily records should be analyzed to determine appropriate regional models of the ARMA type for various quality constituents.

3. Techniques should be explored for the design of monitoring networks based on daily records of flow or total dissolved solids supplemented with sparser records of other quality constituents. Such techniques would be based on the cross correlation between flow or total dissolved solids and other quality constituents.

4. "Cookbook" network design and data analysis packages that include well-documented Fortran or programmable calculator programs should be prepared and distributed to regulatory agencies (or made available through STORET). These packages should provide the capability of estimating deterministic components from data records, computing confidence interval widths about annual means and geometric means for time series of various correlation structures, and assigning sampling frequencies throughout a network via mathematical programming.

SECTION 4

REVIEW OF LITERATURE

Much has been written in recent years on the subject of water quality monitoring, and adequate literature reviews that summarize the work reported up to 1976 have also appeared. Such a summary will not be repeated here, but those major reports prior to 1976 that form the basis for the current project will be discussed. The literature reviews will be identified, and pertinent publications that have appeared since 1976 will be pointed out.

The first portion of this literature review covers material of a general nature dealing with nationwide needs for water quality data in support of water quality management and the degree to which those needs are or are not being met. The rest of the review covers material dealing with the more technical considerations of designing water quality monitoring networks, particularly the assignment of sampling frequencies. First, early approaches to design with the objective of detecting pollution events are mentioned. Then more currently applicable approaches with the objective of determining annual means and using fairly basic statistical methods are reviewed. Turning to the more complex problem of determining annual means while considering serial correlation, the necessary background material is covered next. Finally, advanced design approaches that make use of this theory are reviewed.

MONITORING POLICY AND EVALUATION

Several reports have attempted to describe the state of water quality monitoring in general terms and to identify specific problems and deficiencies in current monitoring practices. Foremost among these is the National Research Council of the National Academy of Sciences (1977) report entitled "Environmental Monitoring." This report was prepared for the U.S. Environmental Protection Agency (EPA) at the request of the U.S. Congress and deals with monitoring programs both operated and supervised by EPA. The latter would include regulatory monitoring by State water quality authorities. Many of the conclusions and recommendations of this report underscore the need for performing research of the type described here. Among the pertinent conclusions are the following:

1. The objectives of monitoring programs should be more clearly defined.

2. An effort should be made to better incorporate scientific principles (including statistics) into the design, evaluation, and operation of monitoring systems.

3. The design of monitoring networks should incorporate an analysis of the trade-offs between cost and effectiveness.

4. Data collected through monitoring efforts should be more thoroughly analyzed with respect to the intended use, adequately summarized, and more widely disseminated.

5. Decisions in environmental management should rely more heavily on data collected in the past.

A more detailed summary of the National Academy of Sciences report is presented by Kendrick (1977).

An interesting philosophical treatise on designing hydrologic data collection networks is given by Moss et al. (1978). The paper includes a restatement of an obvious, but sometimes forgotten, problem of design. Namely, if enough information were known about the hydrologic phenomena involved to perfectly design a network, there would be no need to collect additional data. The need for further research into hydrologic network design is emphasized, particularly with respect to careful definition of monitoring objectives, determining the value of data obtained from monitoring, and relating monitoring network design to data utilization.

Cleary (1978) makes this crucial point regarding the role of background data in water quality management decisions:

> Before billions of dollars are spent for measures to control the quality of U.S. rivers, their elusive aspects should be understood. Unfortunately those who try to understand--those responsible for forming public policy and deciding how those billions of dollars will be spent--face a serious handicap. That handicap is a lack of information describing past river quality and reasons for the variability in that quality.

Cleary recognizes the National Stream Quality Accounting Network (NASQAN) established by the U.S. Geological Survey in 1972 as having the greatest promise for improving the nationwide water quality data base. A description of the NASQAN program is presented in Cragwall (1976), and summarized results of the program, which attempt to describe the current state of national water quality on a region-by-region basis, are available in Steele et al. (1974), Hawkinson et al. (1977), and Briggs and Ficke (1978).

The NASQAN system is dedicated to detecting long-term changes in stream quality on a nationwide basis. Therefore, station locations are chosen to account for as much of the Nation's streamflow as possible, and uniform sampling frequencies for several constituents are used throughout the network (Hawkinson and Ficke, 1975).

Why then are States required to operate their own monitoring networks, and why should a State network be subject to different design criteria than NASQAN? The State water quality authorities must make management decisions on a short-term basis (crisis-oriented management) and must have water quality data that is tailored to this purpose. For example, biannual reports

on the current condition of water quality in the State are required by Section 305-B of the Clean Water Act. Therefore, annual means (yearly averages) of pertinent water quality variables are meaningful statistics for this short-term type of management strategy. The confidence interval approach to design, to be discussed later, allows States to allocate their limited monitoring resources among stations in order to gain the largest possible amount of usable information for a given level of expenditure. It further facilitates an understanding of the significance of changes from year to year of annual means in water quality.

The emphasis in regulatory monitoring has traditionally been directed toward assessing the effectiveness of municipal or point-source pollution control. However, the Clean Water Act directs EPA to begin programs to manage and control nonpoint sources. Pisano (1976) discusses Section 208 of the Clean Water Act as the primary legislative mechanism through which States will act to achieve water quality goals via control of both point- and nonpoint-source pollution. Management under Section 208 involves both the planning and implementation of pollution control practices and should be supported through effective monitoring activities. Cooley (1976) provides an editorial comment on some general considerations of monitoring nonpoint-source pollution, including station location and constituent coverage.

A final article that is quite critical of the current approaches to stream quality monitoring is that of Hines et al. (1977) of the U.S. Geological Survey, who state:

> Perhaps justifiably, in light of the complexities involved, enormous amounts of time, money, and effort are spent on river-quality sampling programs. In many basins, however, years of quality sampling have not generated adequate information from which to establish environmental standards or to make sound resource decisions. This situation has resulted in a growing dissatisfaction with river-quality data programs.

These authors suggest an alternative approach to monitoring, consisting of three major elements: (1) increased hydrologic analysis focusing on streamflow, water temperature, channel morphology, and basin history, (2) reinterpretation of existing data in light of the hydrologic analysis, and (3) design of sampling programs based on short-term, synoptic surveys rather than routine monitoring.

The authors indicate, at least indirectly, that this approach would be appropriate for regulatory objectives (environmental decisions); however, many of the practical realities of monitoring at the State level, such as a dearth of expertise in water quality hydrology, are ignored. Also, the intensive survey approach has been shown by Lettenmaier (1978) to be less than satisfactory for trend detection; this will be covered later. Thus it is apparent that much disagreement exists among experts as to what the basic nature of monitoring programs should be.

TECHNICAL APPROACHES TO DESIGN

Detecting Pollution Events

Within the past six years, several major reports have appeared that address the technical aspects of the design of monitoring systems for water quality management purposes. Although each includes a statistical approach to the design problem, they differ widely in their objectives and recommended methods.

In the late 1960's and early 1970's when water quality management was guided by the Federal Water Quality Act of 1965 (PL 89-234), it was thought that stream quality monitoring should have as its goal the detection of stream standard violations (pollution events). Ward (1973) proposed a monitoring network design that would include two classes of stations. A primary network would be designed to detect stream standard violations, and a secondary network would be designed to detect trends. The primary network would be designed using a simulation model to determine the effectiveness of a monitoring scheme in detecting pollutant spills. The secondary network would be designed to determine annual means of river quality constituents with a given width of confidence interval. In each case costs would be balanced against effectiveness.

Beckers and Chamberlain (1974) presented a more sophisticated approach to designing for detecting stream standard violations. They developed a complete, computerized design package using more complex stream models and more detailed cost-effectiveness analyses than were applied by Ward (1973).

With time the realization of two important factors led to a shift away from the objective of detecting stream standard violations. The first factor is that such networks require high sampling frequencies and thus high costs to operate with any satisfactory level of performance. The second is that effluent monitoring became recognized (as a result of the 1972 Federal Water Pollution Control Act Amendments, PL 92-500) as the only practical way to enforce pollution standards.

Determining Annual Means

Thus the emphasis in stream monitoring has now been placed on the determination of annual means and trends of various water quality constituents. Montgomery and Hart (1974) and Sherwani and Moreau (1975) provide reviews of basic statistical techniques that may be applied to the design of such a network.

Ward et al. (1976) provide an excellent summary of those statistical tools that might possibly be adopted by regulatory agencies within the near future. The emphasis is placed on the basic statistics of the water quality "population" such as the annual mean and variance. Design of sampling frequencies in order to achieve desired widths of confidence intervals about annual means is discussed. Stratified sampling and linear programming are suggested as appropriate design tools. In addition, a comprehensive review of literature is presented, which adequately presents the state of the art in water quality monitoring at the time of publication. In a concluding section, the relationship of data needs and data utilization by agencies to their selection of monitoring strategies is discussed.

An additional population statistic of importance in water quality, which is often used in place of the annual mean, is the geometric mean. The geometric mean of flow is important in the work of Sanders (1974). The properties of the geometric mean in the context of its use in water quality standards are further discussed in Landwehr (1978).

The arguments of Sanders and Ward (1978) point out that the full value of any statistical approach to the design of monitoring networks can only be realized if State governments are willing to incorporate these same statistics into water quality decisions such as the setting of stream standards and defining standards violations.

Considering Serial Correlation

A major limitation of the work of Ward et al. (1976) would appear to be the assumption that, in most water quality sampling for regulatory purposes, the samples will be independent. The extension of the same statistical concepts to the case of samples that are not independent but serially correlated requires that the field of time series analysis be introduced into the subject of monitoring design. The basic statistical concepts involved in this extension are illustrated in the following papers.

Bourodimos et al. (1974) examine the stochastic nature of water quality time series--specifically, streamflow, temperature, dissolved oxygen, and biochemical oxygen demand. These time series are assumed to consist of three components: (1) a trend; (2) a cyclic or seasonal component; and (3) irregular fluctuations or a random component. The trend component is modeled by a polynomial, and the cyclic component by a sinusoidal expression. The random component is studied through its autocorrelation and spectral density functions. The essential concept, though, is that of viewing a water quality time series as composed of deterministic and stochastic portions that may be isolated and studied independently. This concept is also applied elsewhere in the literature, for example in Steele et al. (1974) and in Sanders (1974).

The stochastic component of a water quality time series will in general be serially correlated. The importance of this phenomenon relative to monitoring is explicitly conveyed in Matalas and Langbein (1962) in the following statement.

> Hydrologic series frequently consist of observations that are dependent on one another. Such series are referred to as nonrandom series and may be represented by a simple Markov model. The dependence between the observations is measured by the autocorrelation coefficients. In a nonrandom series each observation repeats part of the information contained in past observations. Consequently a nonrandom series yields less information about the mean than a random series having an equal number of observations.

The means by which this reduction in information may be quantified mathematically will be developed in detail in Section 5.

The use of the first-order Markov model is illustrated in Rodriguez-Iturbe (1969) as applied to annual river flow. This simple stochastic model

expresses the present value of a time series in terms of the immediately preceding value and a random shock or uncorrelated noise term. The only parameters of this model are the lag-one autocorrelation coefficient and the mean and variance of the series. Rodriguez-Iturbe discusses the range of errors involved in estimating these parameters for annual river flows, indicating that large errors may result when fewer than 40 observations are used in estimation.

The lag-one Markov model is a member of a larger class of time series models known as autoregressive, moving-average (ARMA) models. The classic text that covers this type of model is Box and Jenkins (1976). This text is the basis for all of the time series analyses performed in connection with the research described here.

Box-Jenkins type time series analysis has become extremely popular in recent years, and journal articles have appeared describing the application of ARMA models to many types of time series. An interesting study in which time series models of the ARMA type were constructed for water temperature and flow and then used for forecasting is described in McMichael and Hunter (1972). A significant portion of the paper is devoted to introducing the work of Box and Jenkins and describing the process of model construction.

The process of model construction has been refined since the appearance of Box and Jenkins. These developments have been published in articles such as Hipel et al. (1977) and McLeod et al. (1977). The first article includes a summary of model identification, parameter estimation, and diagnostic checks. The second paper includes application to three actual time series, each of which is a "classic" that had been modeled and discussed previously.

Advances in ARMA modeling occur so rapidly that it is difficult to define the state of the art at any one time. The British journal Biometrika is a good source of information concerning the latest developments in model construction, but the level of presentation is suitable for reading primarily by statisticians. On a more practical level, the method by which one constructs a time series model will usually depend on the availability of computer programs to perform this function.

Advanced Design Techniques

Two reports have appeared that view water quality observations as serially correlated time series. Sanders (1974) studied the turbulent diffusion of a conservative pollutant to establish mixing length criteria for sampling station location. Sampling frequencies were determined based on daily observations of flow. Time series analysis was used to isolate the residual random noise component of flow data, and then sampling frequencies were assigned to achieve a given confidence interval width for the noise term. This work represents the first attempt to take the confidence interval approach beyond the simple situation of independent samples to cases where serial correlation is important. The portion of the work dealing with the assignment of sampling frequencies is summarized in Sanders and Adrian (1978).

Lettenmaier (1975) presented a rather sophisticated approach to designing

a network for trend detection. He discussed two major points: (1) the power of nonparametric tests for detecting linear and step trends in equally spaced, serially correlated water quality observations, and (2) coupling statistics and water quality models to determine spatial location of sampling stations such that the average power of trend detection would be a maximum. Both Sanders (1974) and Lettenmaier (1975) include excellent reviews of the literature of water quality monitoring.

Two important papers supporting the above work are Lettenmaier and Burges (1976a) and Lettenmaier (1976). The former paper is a summary of the complete report, and the latter paper is a discussion of nonparametric statistical tests for trend that can be applied to water quality records. Procedures are described for assigning sampling frequencies in order to achieve desired power of trend detection for either a linear or step trend. Many of the specific results are dependent on the assumption that a simple Markov (first-order autoregressive) model adequately describes most water quality time series.

The most recent in this series of articles (and the most relevant to this current research) is Lettenmaier (1978). This article deals further with the problem of designing networks for trend detection. Specifically the power of trend detection tests in the case of constant sampling frequencies is compared to that for stratified sampling (sampling one year in three). The conclusion is reached that constant sampling frequencies are superior for trend detection even when two or three times as many samples may be collected in stratified sampling. The importance of determining the correlation structure of water quality time series for sampling frequency design is emphasized. Subsequently, the difficulty in actually evaluating the correlation coefficients from the type of data records normally available is recognized. A regionalized approach to estimating correlation structure from the few complete records available is suggested. Two other subjects--the use of intervention analysis in trend detection and the geographical location of sampling stations--are briefly touched upon.

There are few reports after Ward et al. (1976) that deal directly with water quality monitoring network design in more specific terms, that is, that spell out exactly how one should set up a sampling program. One notable study, though, is that of Moore et al. (1976). Their research, directed toward monitoring of eutrophication in lakes, produced a cost-effectiveness analysis for assigning sampling frequencies. Using a simple water quality model and estimation theory, the reduction in uncertainty (variance) in the estimates of water quality variables achieved through increased sampling is balanced against the resulting increased cost. The effectiveness of this approach (and many others) is limited by available prior data, adequacy of the water quality model, and the ability of the designer to place a value on the reduction of uncertainty in estimates. An additional drawback, with regard to application by State agencies, is that the necessary statistical and mathematical theory is far beyond the capabilities of existing agency personnel. This limitation is shared with the design approach presented by Lettenmaier (1975) and is one of the more serious problems associated with upgrading monitoring programs at the State level.

SECTION 5

STATISTICAL ANALYSIS OF HISTORIC DATA

BASIC STATISTICAL CONCEPTS

Confidence Interval About Mean

The value (concentration) of a water quality constituent is a function of time, represented as X_t. The annual mean concentration of the constituent is precisely:

$$\mu = \frac{1}{T} \int_0^T X_t \, dt$$

where T is the period of consideration, in this case one year. The mean is estimated from discrete grab samples as a sum:

$$\mu \simeq \overline{X}_T = \frac{\sum_{t=1}^{k} X_t}{k} \qquad (1)$$

where k is the number of samples collected during period T and $k = T/\Delta t$, where Δt is the interval between samples (assumed equal).

Another parameter for characterizing water quality "populations" and the one that is primarily used in this research is the geometric mean. The geometric mean μ' is estimated from:

$$\mu' \simeq \overline{X}'_T = \exp\left[\frac{\sum_{t=1}^{k} \ln X_t}{k}\right] = \frac{\prod_{t=1}^{k} X_t}{k}$$

Here $\overline{X}'_T$ is the sample geometric mean. The geometric mean is simply the quantity that results from dealing with the logarithms of the water quality observations rather than the raw observations.

The geometric mean is probably a more useful statistic of water quality random variables in general than is the mean for several reasons. One reason is that the logarithms of water quality observations are often more nearly normally distributed than are the observations themselves. In this case, the geometric mean more closely approximates the median than does the mean. Water quality observations for a single constituent may range over orders of

magnitude. If only a few observations are taken, the mean will be heavily influenced by a single large observed value. The geometric mean will be less influenced by the large value and will provide a more meaningful indication of central tendency. Finally, water quality time series composed of logs of observations will be free of the very large fluctuation in magnitudes of observations found in most untransformed series. Thus because the logarithmic series are better behaved, they can be modeled more effectively.

If the population variance is known, a $(1 - \alpha) \times 100$ percent confidence interval about the sample mean is given by:

$$\left\{ \bar{X} - (K_{\alpha/2})[\mathrm{var}(\bar{X})]^{1/2} \quad , \quad \bar{X} + (K_{\alpha/2})[\mathrm{var}(\bar{X})]^{1/2} \right\} \tag{2}$$

where $\mathrm{var}(\bar{X})$ = the variance of the sample mean

$K_{\alpha/2}$ = the standard normal deviance corresponding to a probability of $\alpha/2$ (tabulated)

$(1 - \alpha) \times 100\%$ = significance level

A 95 percent confidence interval may be defined by the following probability statement: There is a 95 percent probability that the true mean lies within the interval about the sample mean given by (2) above.

The above holds if the sample mean is normally distributed. The Central Limit Theorem indicates that this will usually be true for sample sizes greater than 10 (Bendat and Piersol, 1971).

If the observations are independent, the variance of the sample mean is given by:

$$\mathrm{var}(\bar{X}) = \frac{\sigma^2}{k} \tag{3}$$

where σ^2 = the population variance

k = number of observations

In this case it is a simple matter to compute the number of observations (k) necessary to achieve a confidence interval of a particular width. Let one-half the desired width of the confidence interval be represented by R, where:

$$R = K_{\alpha/2} \frac{\sigma}{\sqrt{k}}$$

Thus:

$$k = \left[\frac{K_{\alpha/2}\, \sigma}{R} \right]^2 \tag{4}$$

This procedure is applied to water quality sampling in Ward et al. (1976).

If, on the other hand, the observations are not independent, the variance of the sample mean is larger than σ^2/k and the above procedure will result in a sample size that is smaller than that actually required. This problem may be handled as follows.

A serially correlated time series of water quality observations may be written as a sum of deterministic and stochastic components: $X_t = y_t + Z_t$.

where X_t = the value of the observation at time t

y_t = the value of the deterministic component at time t

Z_t = the value of the stochastic component at time t (Z_t must be stationary)

In general, both X_t and Z_t will be serially correlated.

In order to determine a confidence interval about the sample mean, it is necessary to develop an expression for $\text{var}(\bar{X})$:

$$\text{var}(\bar{X}) = \text{var}\left[\frac{1}{k}\sum_{t=0}^{k-1} X_t\right]$$

$$= \text{var}\left[\frac{1}{k}\sum_{t=0}^{k-1} (y_t + Z_t)\right]$$

Since there is no variance associated with the y_t terms, we have:

$$\text{var}(\bar{X}) = \frac{1}{k^2}\left[\sum_{i=0}^{k-1}\sum_{j=0}^{k-1} \text{cov}(Z_{t+i}, Z_{t+j})\right]$$

$$= \frac{\sigma_z^2}{k^2}\left[k + 2(k-1)\rho(1) + 2(k-2)\rho(2) + \ldots + 2\rho(k-1)\right]$$

$$= \frac{\sigma_z^2}{k^2}\left[k + 2\sum_{n=1}^{k-1}(k-n)\rho(n)\right] \qquad (5)$$

where $\rho(n)$ = lag-n autocorrelation coefficient

$\sigma_z^2 = \text{var}\,[Z_t]$

Note that equation (5) reduces to equation (2) if the function $\rho(n)$ is zero, which is the case when samples are independent.

If Z_t is stationary:

$$\rho(n) = \frac{\text{cov}[Z_t , Z_{t+n}]}{\text{var}[Z_t]}$$

If y_t is periodic, i.e., X_t is periodic, the sample mean must, of course, be computed over an integral number of periods to have any meaning. In the case of water quality constituents, an annual cycle is commonly exhibited, so the annual mean is a useful statistic. For computing annual means, k in the above derivation corresponds to the number of samples collected in one year and the sampling interval in days would then be $365/k$. Implicit in this discussion is the assumption that:

$$\frac{1}{k} \sum_{k=0}^{k-1} X_t$$

is an unbiased estimator of the annual mean μ, regardless of the point in the deterministic cycle at which the first sample is taken. In order to use equation (5) to compute the variance of the sample mean, it is necessary to know the values of the autocorrelation function of the stochastic component $\rho(n)$: $n = 1, 2, \ldots, k - 1$. These can be estimated from a historic data record; however, one must have considerably more than k data points in order to estimate $k - 1$ autocorrelation coefficients.

A better approach is to fit a time series model to the historic data record with the deterministic component removed and then compute a theoretical autocorrelation function based on that model. This will generally require less data and, it is hoped, will result in an autocorrelation function that is "smoother" and more representative of the underlying stochastic process than an autocorrelation function estimated from a particular realization of the process.

ARMA Models

The general class of time series models used for this purpose is autoregressive, moving average (ARMA) models as described in Box and Jenkins (1976).

An ARMA (p,q) model possesses the following form:

$$Z_t = \phi_1 Z_{t-1} + \phi_2 Z_{t-2} + \ldots + \phi_p Z_{t-p} + a_t$$

$$- \theta_1 a_{t-1} - \theta_2 a_{t-2} + \ldots - \theta_q a_{t-q} \qquad (6)$$

where Z_t = present value of the time series

Z_{t-1} = value of the series one time interval in the past, etc.

$\phi_1, \phi_2, \ldots, \phi_p$ = autoregressive coefficients

$\theta_1, \theta_2, \ldots, \theta_p$ = moving-average coefficients

a_t = present value of a random noise term or "shock"

a_{t-1} = value of random shock at time t-1

The model expresses the current value of the time series in terms of previous values, a random shock, and previous values of the random shock. One effect of the model is to remove all serial correlation from the time series, reducing it to a series of independent noise terms or shocks, a_t. The variance of the residuals, σ_a^2, will be less than the variance of the time series, σ_a^2, since the variance of the time series includes the effect of correlation. In a purely autoregressive model, AR(p), all of the moving-average coefficients are zero. Likewise in a purely moving-average model, MA(q), all of the autoregressive coefficients are zero.

A particular ARMA (p, q) process with specified coefficients will have a unique autocorrelation function associated with it. This function may then be used to determine the variance of the sample mean for equally spaced samples drawn from the process. The sampling frequency necessary to achieve a specified confidence interval that accounts for the effect of serial correlation may then be determined by computing the variance of the sample mean and width of the confidence interval for various sample sizes and selecting the appropriate one.

The autocorrelation function desired is that of the stochastic component only. Therefore, the deterministic component must be removed before a time series model is fitted. For this research, the deterministic component was assumed to consist of a linear trend plus a sinusoidal component with a period of one year. This deterministic function has the form:

$$y_t = mt + A(\cos wt + C) \tag{7}$$

where y_t = deterministic component at time t

w = 360 degrees/number of samples per year

m, A, C = fitted constants

A similar form of the deterministic function is also applied in Sanders (1974) and in Steele et al. (1974).

APPLICATION

Data Records Used

Water quality records from three locations were analyzed using the methods described above to determine their correlation structures. For

selected constituents a range of hypothetical sampling frequencies were then assigned, confidence intervals were computed, and the results were compared with those obtained when serial correlation was not considered. The water quality records used were:

1. Approximately two years of weekly observations for four constituents from the Red River at Emerson, Manitoba. The period of record considered was August 1960 through June 1962. Constituents considered were specific conductance, sodium, bicarbonate, and chloride.

2. Approximately 15 months of daily observations for four constituents from the Grand River at 68th Avenue Bridge, Allendale, Michigan. Period of record considered was March 1, 1976, through April 30, 1977. Constituents considered were specific conductance, total phosphate, sulfate, and chloride.

3. One year of daily observations for five constituents at each of nine stations in Illinois. Constituents considered were total dissolved solids, total organic carbon, suspended solids, total hardness, nitrates, and turbidity.

Data were obtained from the Monitoring and Surveys Division, Water Quality Branch, Inland Waters Directorate, Ottawa, Canada; from the U. S. Environmental Protection Agency, Region V, Chicago, Illinois; and from the Illinois State Water Survey, Urbana, Illinois, respectively.

The data sets from the Canadian and Michigan locations were evaluated first and used to gain experience in model fitting. (The results from these two locations are presented first to describe the fitting process.) The model fitting procedure was therefore more "streamlined" and efficient when the much larger task of working with records from an entire network in Illinois was begun.

For each of the Michigan data records, the parameters m, A, and C in equation (7) were fitted by the method of least squares as described in Sanders (1974), and then the function y_t was subtracted from the data record before an ARMA model was fitted.

In practice, it would be unwise to estimate a linear trend based on a single year of observations. Therefore the linear trend was not removed from the Canadian or Illinois time series that were used in the final design example. If, however, longer historic records were available, one would normally estimate a linear trend component and then apply a statistical test to see if it were significant. A "t" test--as described in any basic statistics text such as Bowler and Lieberman (1972)--strictly applies only if the individual observations are independent and identically, normally distributed, but it may be useful also when these conditions "roughly" hold. Modified "t" tests for records with dependent observations and nonparametric tests (which are not based on a probability distribution) for trend are given by Lettenmaier (1976, 1978).

The deterministic coefficients that were estimated for the seasonal components of the water quality time series under study are listed in the Appendix.

Time series models of the ARMA type were fitted to each data record using the IMSL (International Mathematics and Statistics Library) subroutines and the Control Data Corporation CYBER 172 computer system at Colorado State University.

An initial step in model fitting is often some transformation of the data. In many cases a transformation is selected in order to obtain "better" fits. However, for this research it is important to remember that the models will ultimately be used to generate theoretical autocorrelation functions for time series to be sampled in the future and to establish confidence interval widths about some sample statistic. If the sample statistic of interest were the annual geometric mean, a logarithmic transformation would be used as in Sanders (1974). If the annual mean were of interest, no transformation would be used. For the final design example based on the Illinois data, it is desirable to deal only with geometric means for the sake of consistency, so a logarithmic transformation is used in every case. This rule is followed for the Canadian and Michigan data sets as well. Only models of degree $p \leq 2$ and $q \leq 2$ are considered.

Model Fitting

The process of an ARMA model fitting is rather complex and is perhaps as much an art as a science. A brief description will be attempted here, and a detailed explanation may be found in Box and Jenkins (1970). Likely candidate models are selected based on a visual inspection of autocorrelation and partial autocorrelation functions estimated from the data for the first 20 or so lags. An AR(p) process tends to exhibit exponentially decaying or damped sine wave behavior in the autocorrelation function and has a partial autocorrelation function that is zero except for the first p values. A moving average model [MA(q)] would show similar behavior in reverse--exponential decay in the partial autocorrelation function and q nonzero values in the autocorrelation function. Mixed processes tend to exhibit a combination of the above behavioral patterns. The estimated autocorrelation function and partial autocorrelation function for the daily sulfate concentration time series from the Grand River, Michigan, data are shown in Figures 1 and 2. This time series was later fitted by a second-order autoregressive--AR(2)--model.

After likely candidate models are selected, the autoregressive and moving average coefficients are computed by the appropriate IMSL subroutines using the method of maximum likelihood as described in Box and Jenkins (1976). One model is then selected as the best from the various candidates based on an examination of the correlation structure of the residuals and on the magnitude of the residual variance, σ_a^2. If the model were perfect, the residuals would be completely uncorrelated. One would usually select a model that had the smallest residual variance and least correlation remaining among

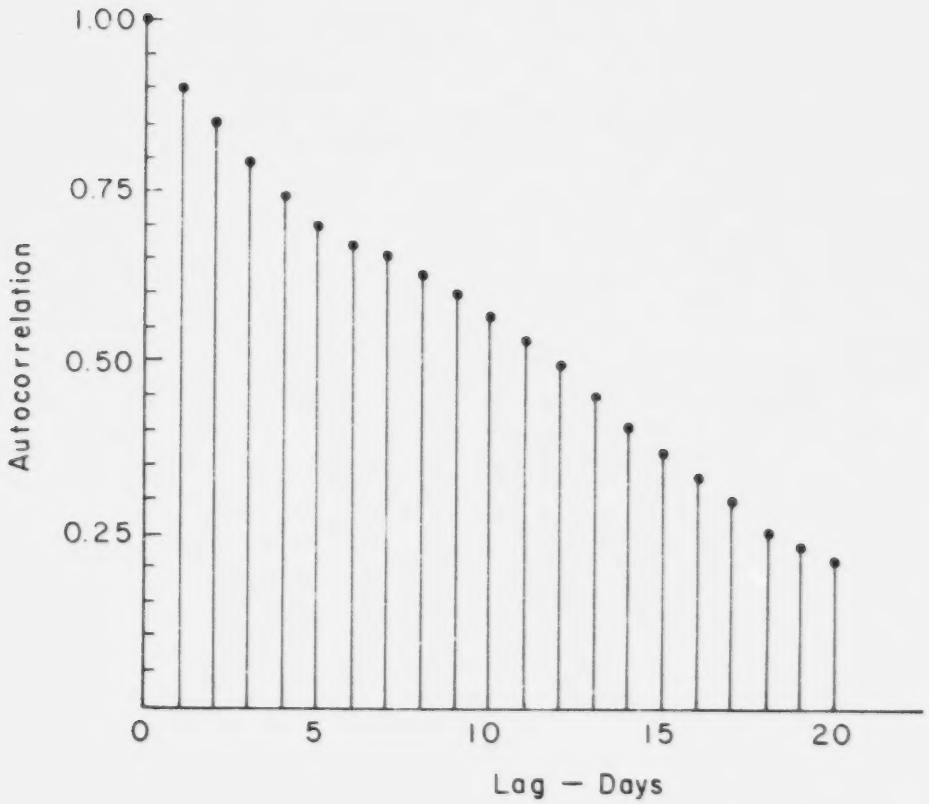

Figure 1. Estimated autocorrelation function for daily sulfate concentration, Grand River, Michigan.

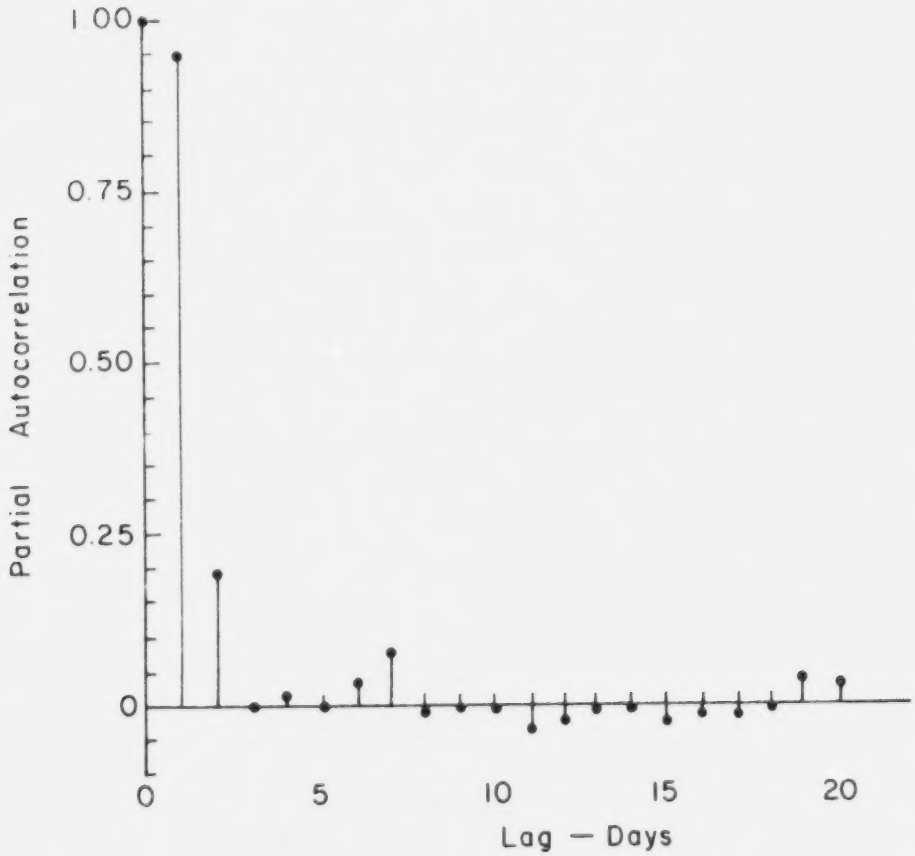

Figure 2. Estimated partial autocorrelation function for daily sulfate concentration, Grand River, Michigan.

the residuals as the best. Other factors must be considered, however. For example, one would like to adopt a model that has as few parameters as possible.

Case Study in Model Fitting

In order to explain the time series model-fitting process in more detail a case study is presented in which the procedures are described step by step. The specific conductance record for the Grand River, Michigan, site is used for this purpose.

After removing the deterministic seasonal component, the first step in model fitting is a visual inspection of the estimated autocorrelation and partial autocorrelation functions. These are given in Figures 3 and 4 and appear very similar to the estimated functions for sulfate concentration in Figures 1 and 2. Since the estimated autocorrelation function decays fairly slowly, a significant autoregressive component is indicated. Only the first two values of the estimated partial autocorrelation function appear to be significant. Therefore, no moving-average component appears to be present, and the autoregressive operator would likely be of degree two. The most likely candidate model, second-order autoregressive, is fitted first using the appropriate IMSL subroutines. Values of the fitted parameters $\phi_1 = 0.63$ and $\phi_2 = 0.28$ result along with a residual variance, σ_a^2, of 0.0026.

The next step is the evaluation of the fitted model. The estimated autocorrelation function $r_k(a)$, of the residuals is shown in Figure 5. According to Box and Jenkins (1970), if the form of the model were known exactly the r_k's of the residuals would be normally distributed with mean zero and standard error $1/\sqrt{n}$. Thus, the standard error limits as shown in Figure 5 may serve as an approximate check on the adequacy of the model. For the current example, the most significant value of r_k occurs at a lag of seven. A logical explanation for this occurrence is that a weekly cycle exists in the time series. A similar occurrence was noted, although to a lesser extent, in other quality series at the same location but was not observed at the other locations. Thus the adequacy of the deterministic model, which should possibly include a weekly component for this location--as suggested by Sanders (1974)--is questionable, but there is little reason to doubt the adequacy of the AR(2) model.

A more quantitative check is given by a test statistic:

$$Q = n \sum_{k=1}^{K} r_k^2(a)$$

where $r_k(a)$ = lag-k autocorrelation coefficient of residuals

n = number of observations to fit the model

K = number of r_k's used in the test (here, $K = 20$)

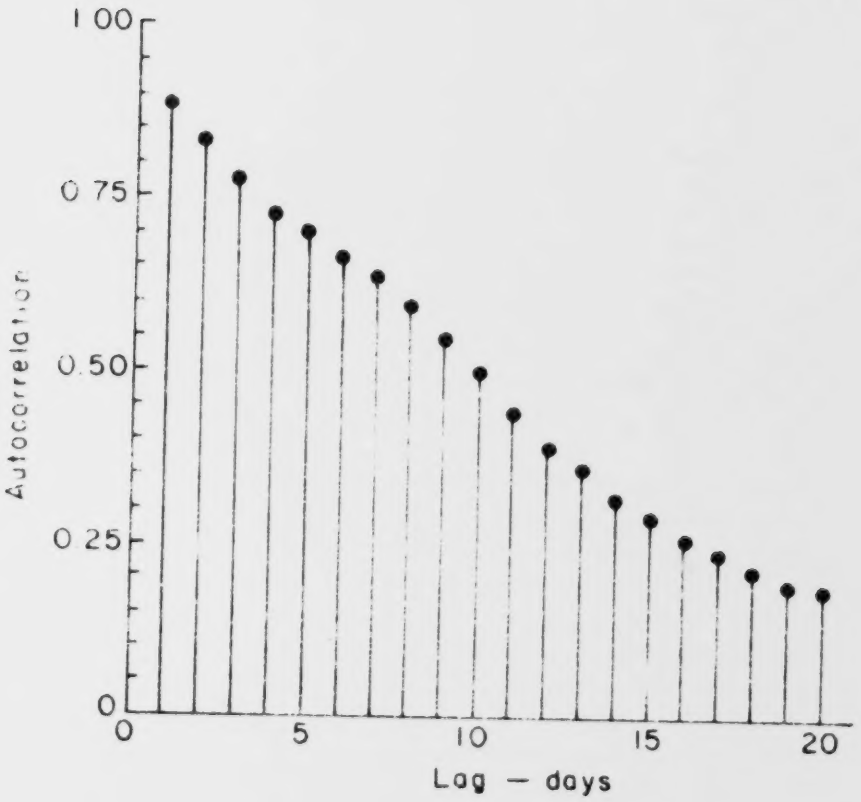

Figure 3. Estimated autocorrelation function for daily specific conductance, Grand River, Michigan.

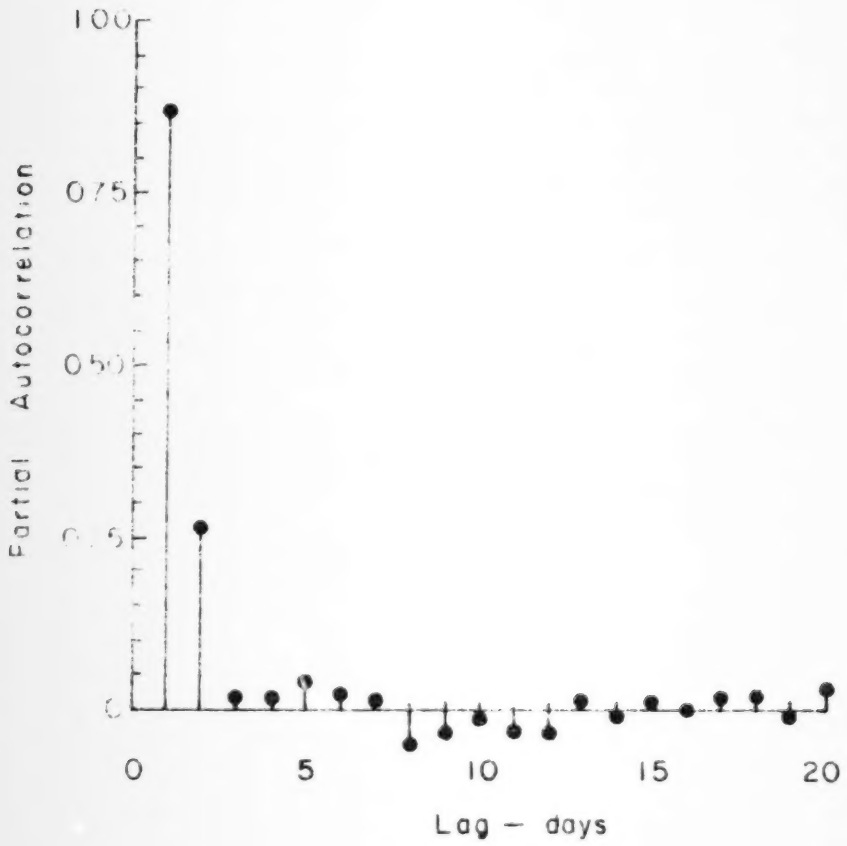

Figure 4. Estimated partial autocorrelation function for daily specific conductance, Grand River, Michigan.

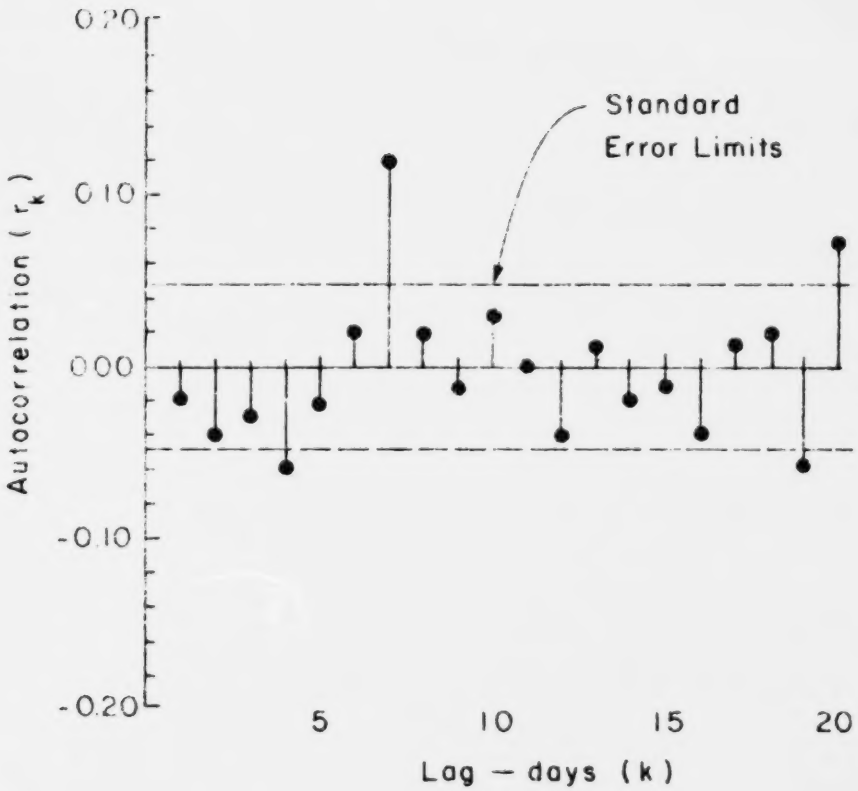

Figure 5. Estimated autocorrelation function of residuals for AR(2) model, specific conductance, Grand River, Michigan.

If the final model is appropriate, Q is approximately distributed as chi-square with (k-p-q) degrees of freedom. Recall, that p and q are the orders of the autoregressive and moving-average components of the model, respectively. By computing α such that the probability that Q is less than χ^2_{k-p-q} equals $1-\alpha$, it is possible to gain some insight into the adequacy of the model. [χ^2_{k-p-q} is the $(1-\alpha)$th quantile of the chi-square distribution with k-p-q degrees of freedom.] One would expect α to be fairly small (say less than 0.10) for adequate models. In practice, however, α may be much larger, particularly when n is large, even when an inspection of the $r_k(\alpha)$ plot would indicate that the model is very good. Therefore, in this research, α was computed primarily for the purpose of comparing models. A model with a smaller α would normally be more acceptable than one with a higher α. For the case study, the fitted AR(2) model results in a value of $\alpha = 0.48$.

A third technique of model evaluation is that of overfitting or fitting more parameters than are actually thought necessary. Thus an AR(3) model is fitted for the case study series. Fitted parameters are $\phi_1 = 0.63$, $\phi_2 = 0.25$, and $\phi_3 = 0.02$. A value of $\alpha = 0.64$ and residual variance (σ_a^2) of 0.0037 are also found. The fact that the value of ϕ_3 is quite small would lend support to the acceptance of an AR(2) model. This conclusion is also supported by the values of α and σ_a^2, which are both larger for the AR(3) model than for the AR(2) model.

Two other candidate models were evaluated, AR(1) and ARMA (2,1). Both appeared to provide poorer fits of the data than did the AR(2) model when measured by the same criteria described above. Thus the AR(2) model was selected. The results of fitting the four candidate models are summarized in Table 1.

TABLE 1. RESULTS OF FITTING CANDIDATE MODELS FOR CONDUCTIVITY TIME SERIES, GRAND RIVER, MICHIGAN

Candidate Model	Fitted Parameters					Chi-Square Significance Level, α
	ϕ_1	ϕ_2	ϕ_3	θ_1	σ_a^2	
AR(1)	0.89				0.0029	0.60
AR(2)	0.63	0.28			0.0026	0.48
AR(3)	0.63	0.25	0.02		0.0037	0.64
ARMA(1,2)	0.70	0.21		0.06	0.0037	0.66

STATISTICAL ANALYSIS RESULTS

Results of Model Fitting

All of the models selected in this study are of the first-order autoregressive, second-order autoregressive, or first-order autoregressive-first-order moving-average types. Tables 2, 3, and 4 indicate the type of model adopted and values of fitted model parameters for each water quality constituent considered for the Manitoba, Michigan, and Illinois locations, respectively. Theoretical autocorrelation functions were computed for each model using the following equations from Box and Jenkins (1976).

For an AR(1) process:

$$\rho_1 = \phi_1 \tag{8}$$

$$\rho_k = \phi_1^k \qquad k = 1, 2, 3, \ldots \tag{9}$$

For an AR(2) process:

$$\rho_1 = \frac{\phi_1}{1-\phi_2} \tag{10}$$

$$\rho_2 = \phi_2 + \frac{\phi_1^2}{1-\phi_2} \tag{11}$$

$$\rho_k = \phi_1\rho_{k-1} + \phi_2\rho_{k-2} \qquad k = 3, 4, 5, \ldots \tag{12}$$

For an ARMA (1,1) process:

$$\rho_1 = \frac{(1 - \theta_1\phi_1)(\phi_1 - \theta_1)}{1 + \theta_1^2 - 2\phi_1\theta_1} \tag{13}$$

$$\rho_k = \phi_1\rho_{k-1} \qquad k = 2, 3, 4, \ldots \tag{14}$$

Theoretical (computed) autocorrelation functions are plotted in Figures 6, 7, 8, and 9 for the Manitoba chloride models, AR(1) process; Manitoba specific conductance model, ARMA(1,1) process; Michigan specific conductance model, AR(2) process; and Michigan total phosphate model, ARMA (1,1) process, respectively. Since each model contains an autoregressive component, all of the autocorrelation functions decay exponentially. However, they differ considerably in the rate of decay.

Computed Confidence Interval Widths For Specific Models

The variance of the sample mean for each water quality constituent was

TABLE 2. RESULTS OF MODEL FITTING, RED RIVER, MANITOBA

Constituent	Model	ϕ_1	ϕ_2	θ_1	σ^2	σ_z^2	μ
log specific conductance (μmhos/cm)	ARMA(1,1)	0.40		-0.37	0.0923	0.567	6.74
log bicarbonate (mg/ℓ)	AR(2)	0.45	0.17		0.145	0.091	5.71
log sodium (mg/ℓ)	AR(1)	0.624			0.350	0.210	3.98
log chloride (mg/ℓ)	AR(1)	0.644			0.602	0.375	4.08

TABLE 3. RESULTS OF MODEL FITTING, GRAND RIVER, MICHIGAN

Constituent	Model	ϕ_1	ϕ_2	θ_1	σ^2	σ_z^2	μ
log specific conductance (μmhos/cm)	AR(2)	0.64	0.28		0.0279	0.0136	6.418
log total phosphate (mg/ℓ)	ARMA(1,1)	0.84		0.10	0.125	0.0953	-1.703
log sulfate (mg/ℓ)	AR(2)	0.4430	0.3771		0.058	0.0169	4.04
log chloride (mg/ℓ)	AR(2)	0.51	0.29		0.130	0.0664	3.661

TABLE 4. RESULTS OF MODEL FITTING, ILLINOIS NETWORK

Constituent*	Model	ϕ_1	ϕ_2	θ_1	σ^2	σ_z^2	μ
		Station #1--Little Wabash River at Louisville, Illinois					
TDS	ARMA(1,1)	0.86		0.03	0.1740	0.1176	5.6793
TOC	AR(1)	0.79			0.1855	0.1833	2.4066
SS	AR(1)	0.86			1.8174	1.1655	3.7091
Hardness	ARMA(1,1)	0.86		-0.02	0.2065	0.1468	5.2670
NO_3^-	AR(1)	0.90			0.6773	0.4276	1.1365
		Station #2--Kankakee River at Kankakee, Illinois					
TDS	AR(1)	0.83			0.00686	0.00600	5.8526
TOC	AR(2)	0.69	0.19		0.1920	0.1298	1.9213
SS	AR(2)	0.73	0.19		1.5596	0.5059	2.6832
Hardness	AR(1)	0.85			0.00948	0.00900	5.7419
NO_3^-	ARMA(1,1)	0.93		-0.14	0.6289	0.5506	1.782
		Station #3--Kankakee River near Lorenzo, Illinois					
TDS	AR(2)	0.65	0.14		0.1658	0.0145	5.8875
TOC	AR(2)	0.61	0.19		0.07536	0.0749	2.0321
SS	AR(2)	0.76	0.11		0.5746	0.5634	3.0103
Hardness	AR(2)	0.69	0.20		0.01744	0.0158	5.6880
NO_3^-	AR(2)	0.53	0.33		0.4649	0.3842	2.2108

*log (mg/ℓ)

(continued)

TABLE 4. (continued)

Constituent*	Model	ϕ_1	ϕ_2	θ_1	σ^2	σ_z^2	μ
	Station #4--Chicago Sanitary and Ship Canal at Lockport, Illinois						
TDS	AR(1)	0.89			0.3292	0.0281	6.0708
TOC	AR(2)	0.38	0.17		0.7536	0.0749	2.3513
SS	AR(2)	0.35	0.21		0.5746	0.5634	3.2369
Hardness	AR(2)	0.74	0.15		0.1639	0.0127	5.3434
NO_3^-	AR(1)	0.56			0.40223	0.2330	2.0266
	Station #5--Illinois River at Ottawa, Illinois						
TDS	ARMA(1,1)	0.85		-0.05	0.01099	0.0105	6.0520
TOC	ARMA(1,1)	0.80		0.10	0.0658	0.0534	2.3383
SS	AR(2)	0.65	0.11		0.4685	0.3311	3.4309
Hardness	AR(1)	0.95			0.01227	0.0116	5.5769
NO_3^-	ARMA(1,1)	0.88		-0.15	0.1619	0.1250	2.553
	Station #6--Vermillion River at Pontiac, Illinois						
TDS	AR(1)	0.96			0.07003	0.0482	6.0069
TOC	AR(2)	0.50	0.20		0.1631	0.1409	2.0488
SS	AR(2)	0.55	0.25		1.3816	0.6979	3.5015
Hardness	AR(1)	0.93			0.07233	0.0583	5.8522
NO_3^-	AR(2)	0.79	0.18		1.8465	1.2864	2.1514

*log(mg/ℓ)

(continued)

TABLE 4. (continued)

Constituent*	Model	ϕ_1	ϕ_2	θ_1	σ^2	σ_z^2	μ
			Station #7--Eureka Lake at Eureka, Illinois				
TDS	AR(2)	0.81	0.16		0.02458	0.0086	5.9165
TOC	AR(2)	0.42	0.45		0.0400	0.0381	2.5203
SS	AR(2)	0.46	0.32		0.3776	0.2270	2.6115
Hardness	AR(1)	0.97			0.02234	0.0105	5.4766
NO_3^-	AR(1)	0.84			1.6920	1.6083	0.2927
			Station #8--Canton Lake at Canton, Illinois				
TDS	AR(1)	0.98			0.0153	0.0061	5.4071
TOC	ARMA(1,1)	0.93		0.15	0.03867	0.0300	1.8897
SS	AR(2)	0.58	0.29		1.0757	0.8078	1.6359
Hardness	AR(1)	0.99			0.02077	0.0082	5.2039
NO_3^-	AR(2)	0.62	0.34		0.6245	0.3458	0.5083
			Station #9--Sangamon River at Lake Decatur, Illinois				
TDS	AR(1)	0.92			0.1169	0.0083	5.7097
TOC	AR(2)	0.46	0.22		0.0801	0.0765	2.0290
SS	AR(2)	0.55	0.24		0.7142	0.2193	2.8744
Hardness	AR(2)	0.86	0.07		0.0146	0.0117	5.5574
NO_3^-	AR(2)	0.41	0.51		2.6655	0.5672	1.6438

*log(mg/ℓ)

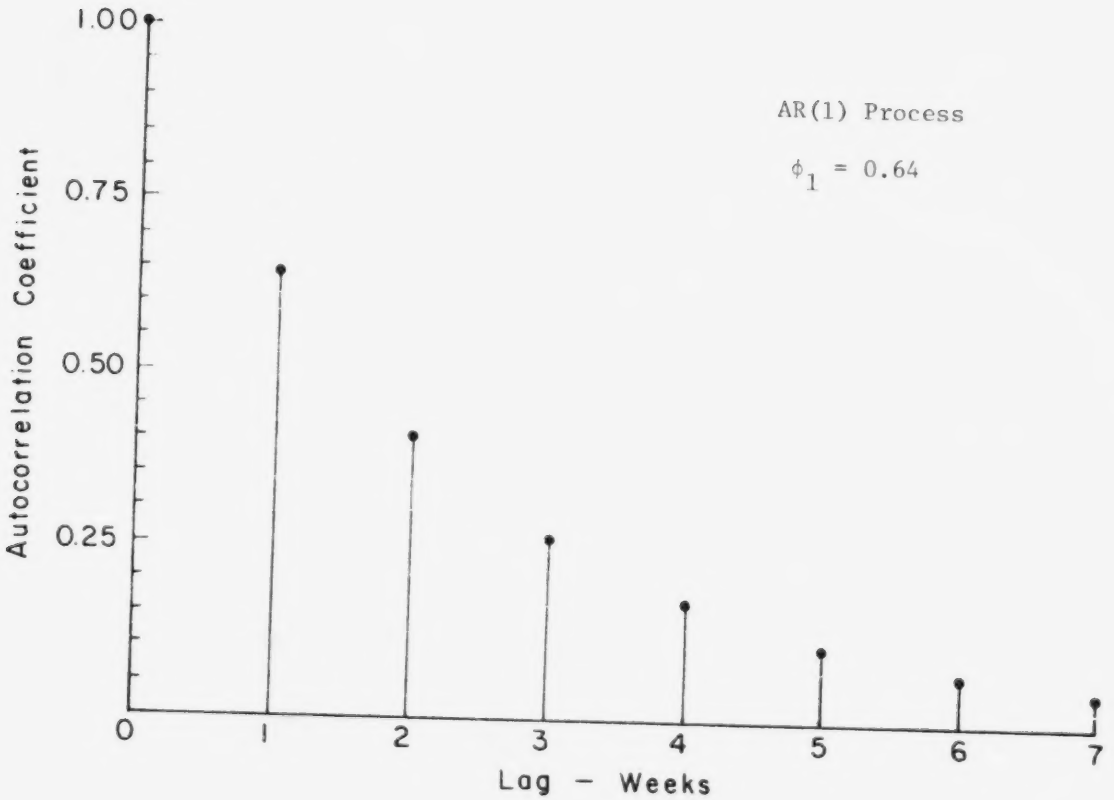

Figure 6. Theoretical autocorrelation function for chloride concentration, Red River, Manitoba.

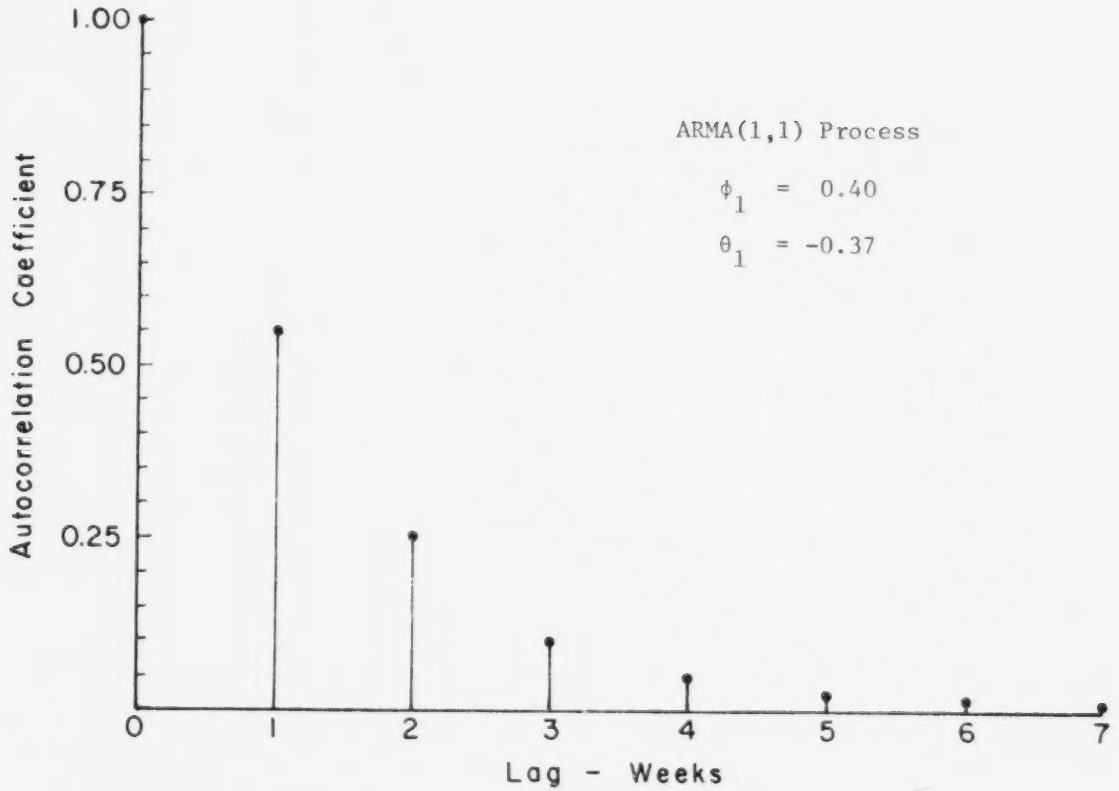

Figure 7. Theoretical autocorrelation function for total phosphate concentration, Red River, Manitoba.

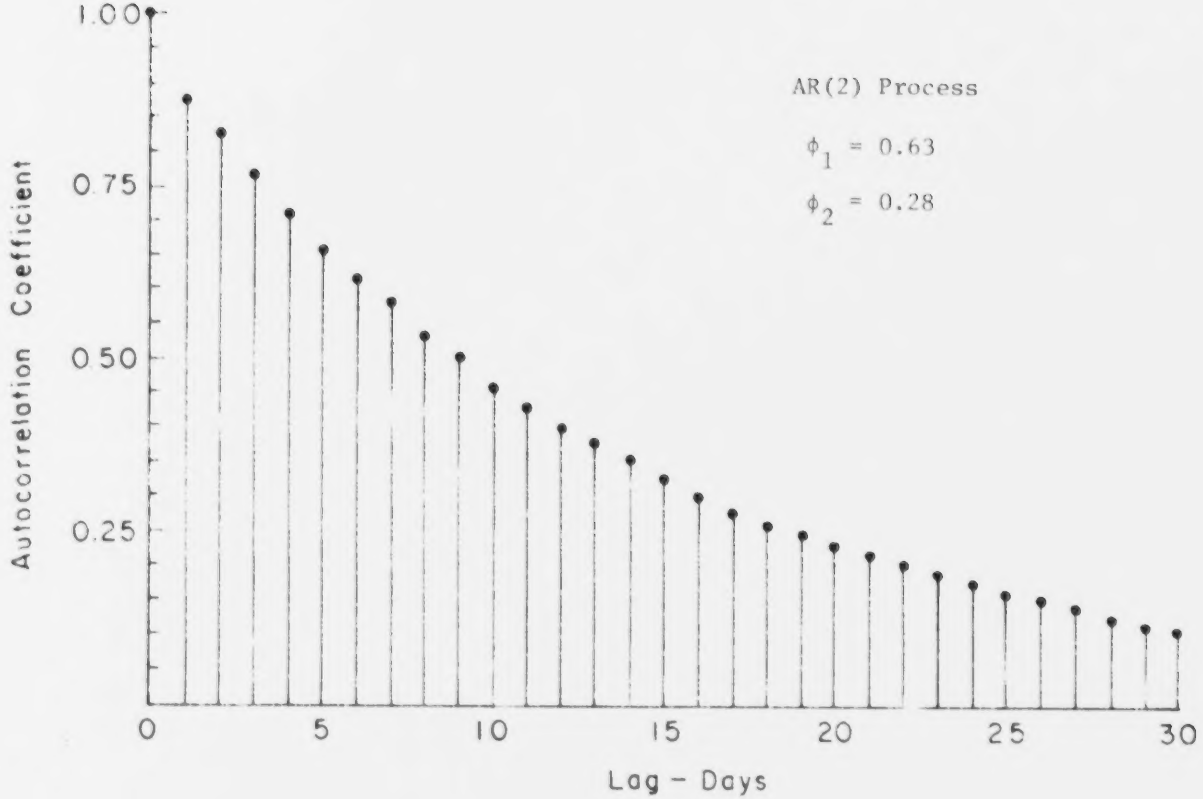

Figure 8. Theoretical autocorrelation function for specific conductance, Grand River, Michigan.

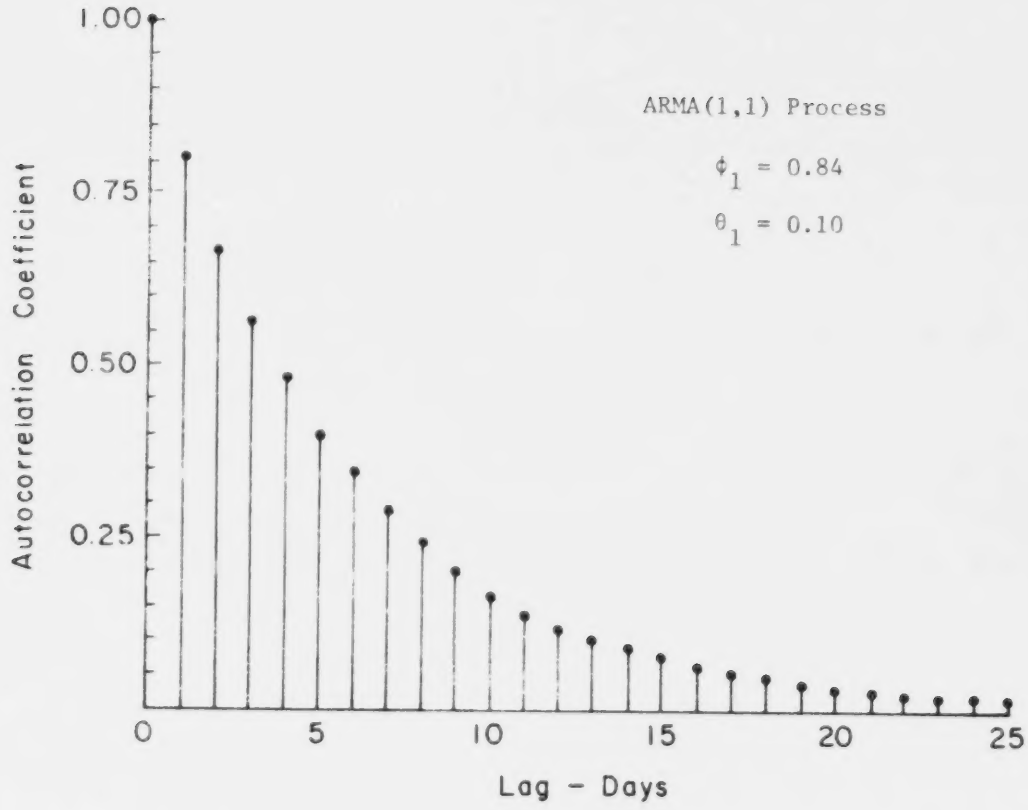

Figure 9. Theoretical authocorrelation function for sulfate concentration, Grand River, Michigan.

then computed over a range of sampling frequencies using equation (5). A 95 percent confidence interval about the sample mean is then:

$$\left\{ \mu - 1.96\ [\mathrm{var}(\bar{X})]^{1/2},\ \ \mu + 1.96\ [\mathrm{var}(\bar{X})]^{1/2} \right\} \tag{15}$$

Since a logarithmic transformation has been performed, the width of the confidence interval about the geometric mean in the original units of the constituent is found from:

$$R = e^{\mu + 1.96[\mathrm{var}(\bar{X})]^{1/2}} - e^{\mu - 1.96[\mathrm{var}(\bar{X})]^{1/2}} \tag{16}$$

The results of these computations for the Canadian and Michigan locations are presented in Table 5. Confidence interval #1 in Table 5 is computed as just described and takes into account both the deterministic component and serial correlation of the time series. Confidence interval #2 is computed from equation (16) using:

$$\mathrm{var}(\bar{X}) = \frac{\sigma_z^2}{k}$$

where k = number of observations per year

σ_z^2 = the variance of the time series with the deterministic component removed

σ_z^2 is estimated from water quality observations from which the function μ_t given by equation (7) has been subtracted. Confidence interval #3 is computed from equation (16) as well, this time using:

$$\mathrm{var}(\bar{X}) = \frac{\sigma^2}{k}$$

as in equation (3), where σ^2 is the variance of the time series without considering either the deterministic component or serial correlation. σ^2 is estimated from the logs of the raw water quality data. Thus confidence intervals #1, #2, and #3 represent successively decreasing levels of sophistication in the analysis.

Since the raw observations contain an apparent (or "false") variance as a result of the deterministic component, confidence interval #2 is always smaller than confidence interval #3. The effect of serial correlation is to increase the variance of the sample mean. Therefore, confidence interval #1 is always larger than confidence interval #2.

When samples are collected frequently, the effect of serial correlation is large and confidence interval #3 is much larger than the other two. However, as the interval between samples increases the effect of serial

TABLE 5. COMPUTED CONFIDENCE INTERVALS* ABOUT GEOMETRIC MEAN FOR SEVERAL WATER QUALITY CONSTITUENTS

Sampling Interval (days)	Width of Confidence Interval #1	Width of Confidence Interval #2	Width of Confidence Interval #3
	Grand River at Allendale, Michigan		
	Specific Conductance (μmhos/cm)		
1	74.3	14.7	21.0
3	74.8	25.5	36.5
7	75.6	38.8	55.7
14	78.5	55.0	78.7
28	87.6	77.8	111.4
36	94.7	88.7	127.1
45	102.5	99.2	142.2
	Total Phosphate (mg/ℓ)		
1	5.4	1.5	2.8
3	5.6	2.6	4.9
7	5.8	4.0	7.5
14	6.5	5.7	10.6
28	8.2	8.1	15.0
36	9.3	9.2	17.1
45	10.3	10.3	19.1
	Sulfate (mg/ℓ)		
1	0.038	0.012	0.013
3	0.039	0.020	0.023
7	0.041	0.031	0.035
14	0.047	0.043	0.050
28	0.062	0.061	0.070
36	0.070	0.070	0.080
45	0.070	0.079	0.090
	Chloride (mg/ℓ)		
1	6.8	2.1	2.9
3	7.0	3.6	5.0
7	7.4	5.5	7.6
14	8.5	7.7	10.8
28	11.0	10.9	15.3
36	12.5	12.5	17.5
45	14.0	14.0	19.6

*Confidence interval #1 accounts for both seasonal and serial correlation effects; confidence interval #2 accounts for seasonal effects only; and confidence interval #3 assumes independent random samples.

(continued)

TABLE 5. (continued)

Sampling Interval (weeks)	Width of Confidence Interval #1	Width of Confidence Interval #2	Width of Confidence Interval #3
	Red River at Emerson, Manitoba		
	Specific Conductance (μmhos/cm)		
1	189.1	109.2	139.4
2	193.2	154.5	197.4
3	209.4	191.3	244.4
4	226.9	218.9	279.7
6	281.0	279.5	357.6
8	323.5	323.2	413.9
	Bicarbonate (mg/ℓ)		
1	105.7	49.6	62.4
2	110.6	70.2	88.4
3	115.8	86.9	109.5
4	120.4	99.5	143.3
6	138.5	127.2	160.6
8	153.0	147.2	186.2
	Sodium (mg/ℓ)		
1	27.2	13.4	17.3
2	28.1	18.9	24.5
3	29.6	23.5	30.4
4	31.0	26.9	35.0
6	36.3	34.5	45.0
8	40.9	40.1	52.5
	Chloride (mg/ℓ)		
1	41.8	19.7	25.0
2	42.9	28.0	35.7
3	45.1	34.8	44.5
4	47.0	40.0	51.2
6	54.9	51.5	66.5
8	61.6	60.0	77.9

*Confidence interval #1 accounts for both seasonal and serial correlation effects; confidence interval #2 accounts for seasonal effects only; and confidence interval #3 assumes independent random samples.

correlation becomes equal to the decrease in variance the results from considering the deterministic annual cycle. For example, this occurs for the Michigan chloride series at a sampling interval of seven days at which point confidence intervals #1 and #3 are equal. At some still larger sampling interval, the effect of serial correlation will disappear entirely. This occurs at about four weeks for the Michigan chloride series at which time confidence intervals #1 and #2 are equal. These relationships are illustrated graphically in Figure 10. Although a design approach using confidence interval #2 is certainly feasible, it is presented here primarily as an intermediate step in arriving at confidence interval #3.

One can readily see that the level of improvement in estimating confidence interval widths that can be gained from the more sophisticated statistical techniques is highly dependent on the sampling interval used and, perhaps to a lesser extent, on the time series model that applies.

Table 6 gives a summary of these results by indicating the relative error of confidence interval #3 as compared to confidence interval #1 for selected sampling frequencies. Taking an average over the four constituents of the Canadian data, confidence interval #3 is 36 percent too narrow in weekly sampling, 12 percent too wide when samples are collected monthly, and 27 percent too wide when samples are collected eight weeks apart. For the Michigan constituents, confidence interval #3 is on the average 61 percent too small in daily sampling, 24 percent too large in biweekly sampling, and 45 percent too large when sampling every 45 days.

One can obtain a better idea of the significance of these results through a simple hypothetical example.

Case 1: Suppose that an agency wishes to monitor the Michigan location in order to determine the annual mean specific conductance with a 95 percent confidence interval width of 40 μmhos/cm. If the simplest statistical approach were used, the agency would implement a program of sampling two times per week (Table 5) but would obtain an "actual" confidence interval width (accounting for the deterministic cycle and serial correlation) of 75 μmhos/cm. If, alternatively, the time series approach described here were used, the agency would realize that the desired confidence interval could not be achieved with daily or less frequent sampling.

Case 2: Now suppose that the desired confidence interval width is 80 μmhos/cm. The agency could adopt biweekly sampling regardless of which statistical approach was used (#1 or #3). Either would be appropriate in this case.

Computed Confidence Interval Widths--Generalized Results

The widths of confidence intervals about the geometric means for five constituents at each station in the Illinois network were computed over a range of sampling frequencies as before. The computed widths were averaged over the nine stations and plotted in Figures 11 through 15 for total dissolved solids, total organic carbon, suspended solids, total hardness, and nitrates, respectively.

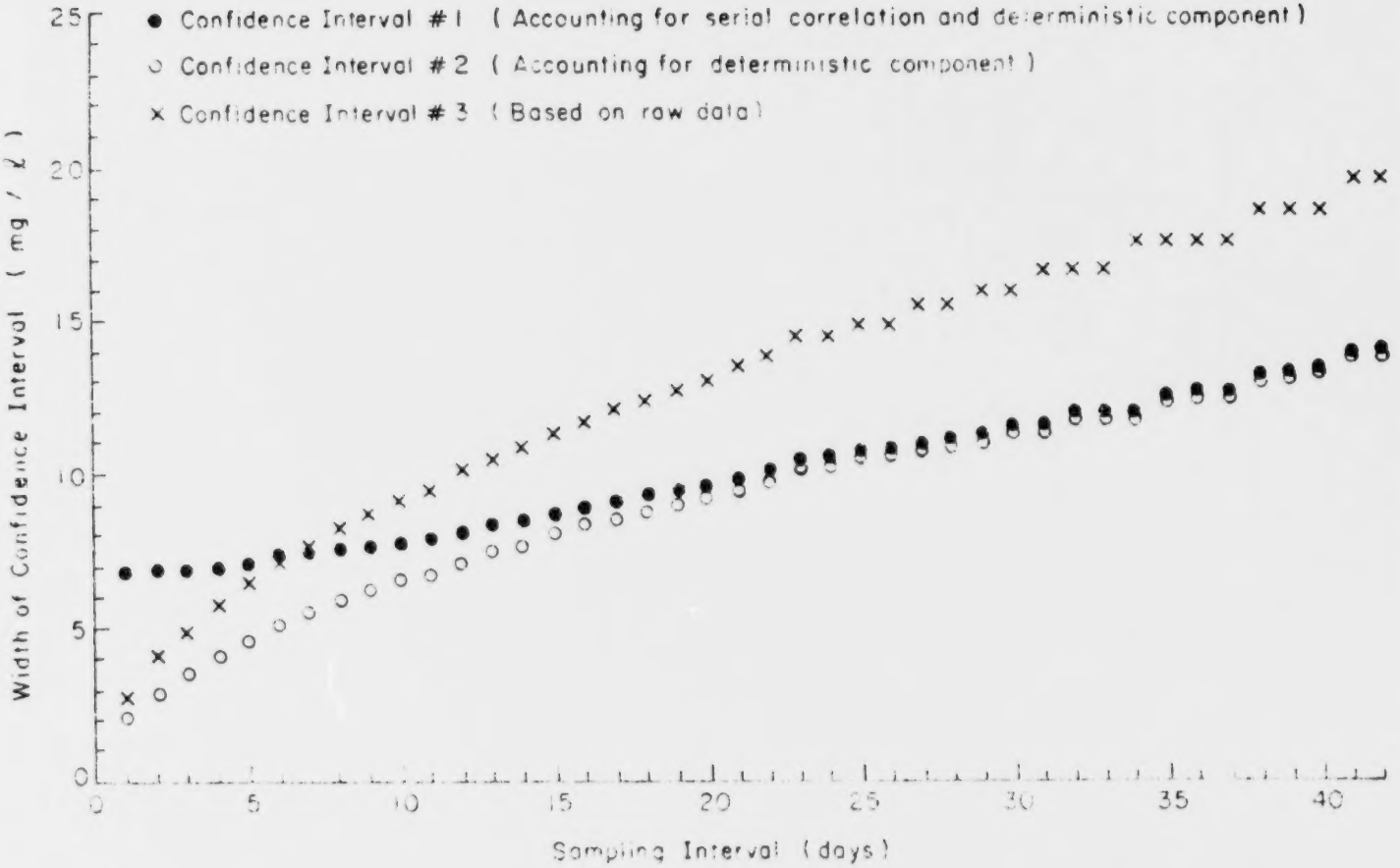
● Confidence Interval # 1 (Accounting for serial correlation and deterministic component)
○ Confidence Interval # 2 (Accounting for deterministic component)
× Confidence Interval # 3 (Based on raw data)
Width of Confidence Interval (mg / ℓ)
Sampling Interval (days)
0
5
10
15
20
25
30
35
40

Figure 10. 95 percent confidence interval widths for the Michigan chloride series as a function of sampling frequency.

TABLE 6. RELATIVE ERROR OF CONFIDENCE INTERVAL #3* AS COMPARED TO CONFIDENCE INTERVAL #1†

Red River, Manitoba				Grand River, Michigan			
	Sampling Interval				Sampling Interval		
Constituent	1 Week	4 Weeks	8 Weeks	Constituent	1 Day	14 Days	45 Days
Conductance	-26%	+23%	+28%	Conductance	-71%	0%	+39%
Bicarbonate	-41%	+ 4%	+22%	Phosphate	-48%	+63%	+85%
Sodium	-37%	+13%	+28%	Sulfate	-66%	+ 6%	+14%
Chloride	-40%	+ 9%	+27%	Chloride	-58%	+28%	+40%
Average	-36%	+12%	+27%	Average	-61%	+24%	+45%

*Confidence interval #3 assumes independent, random samples.

†Confidence interval #1 accounts for effects of serial correlation and seasonal variation.

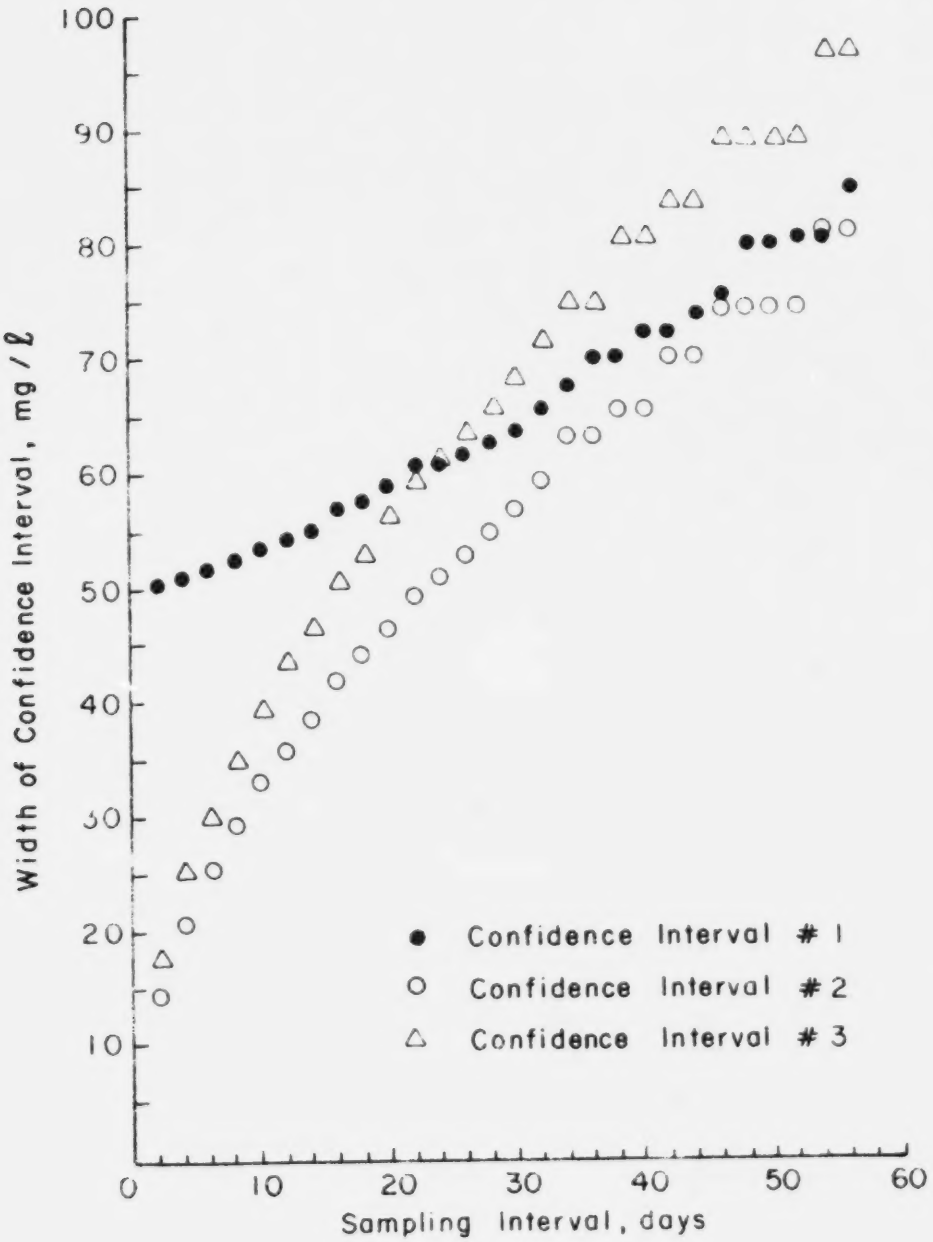

Figure 11. Average 95 percent confidence interval widths about the geometric mean for total dissolved solids in the Illinois network.

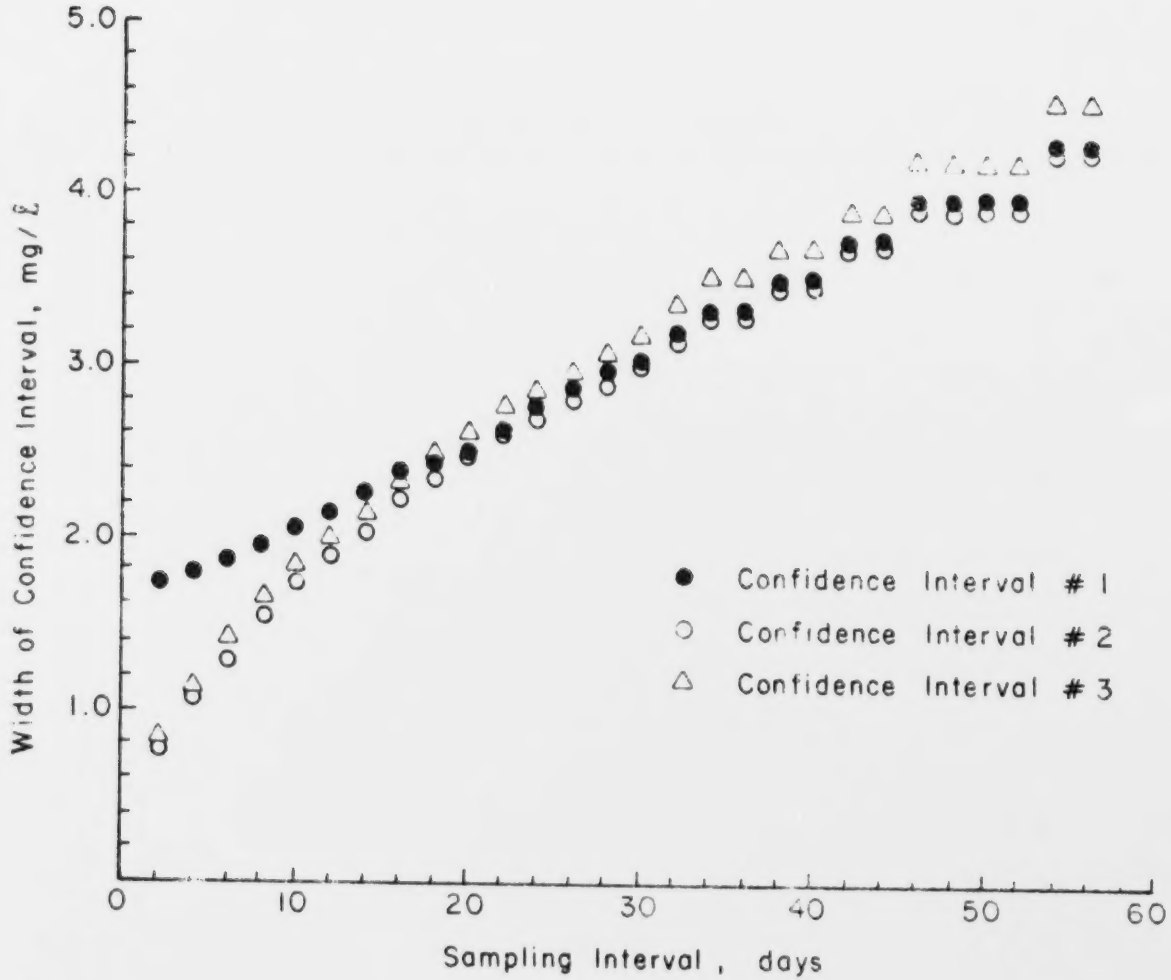

Figure 12. Average 95 percent confidence interval widths about the geometric mean for total organic carbon in the Illinois network.

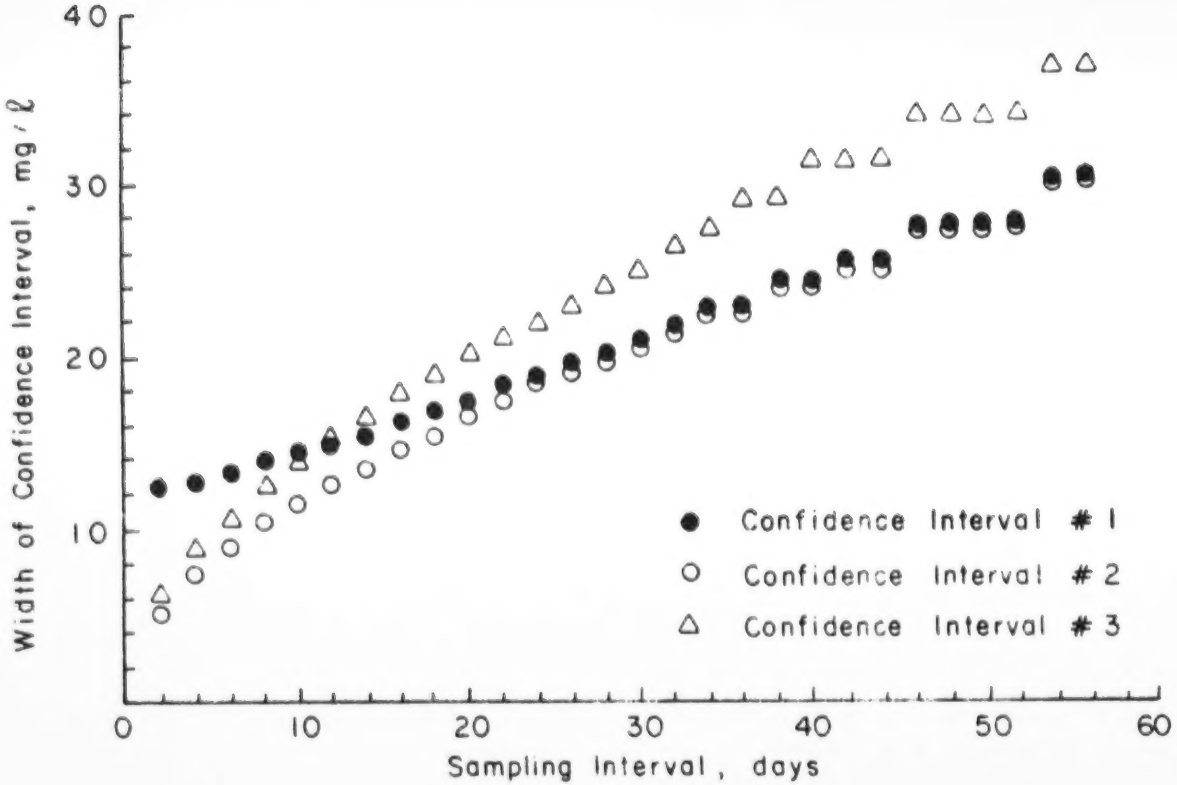

Figure 13. Average 95 percent confidence interval widths about the geometric mean for suspended solids in the Illinois network.

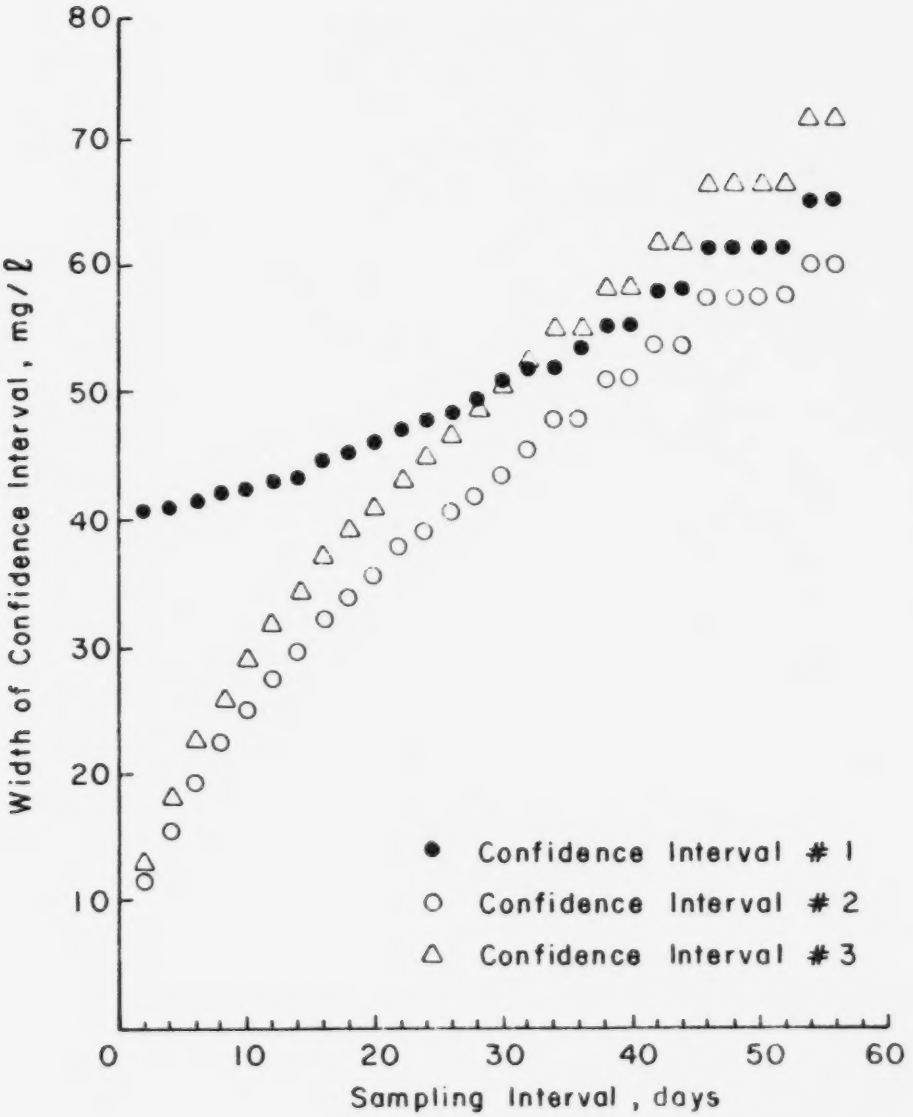

Figure 14. Average 95 percent confidence interval widths about the geometric mean for total hardness in the Illinois network.

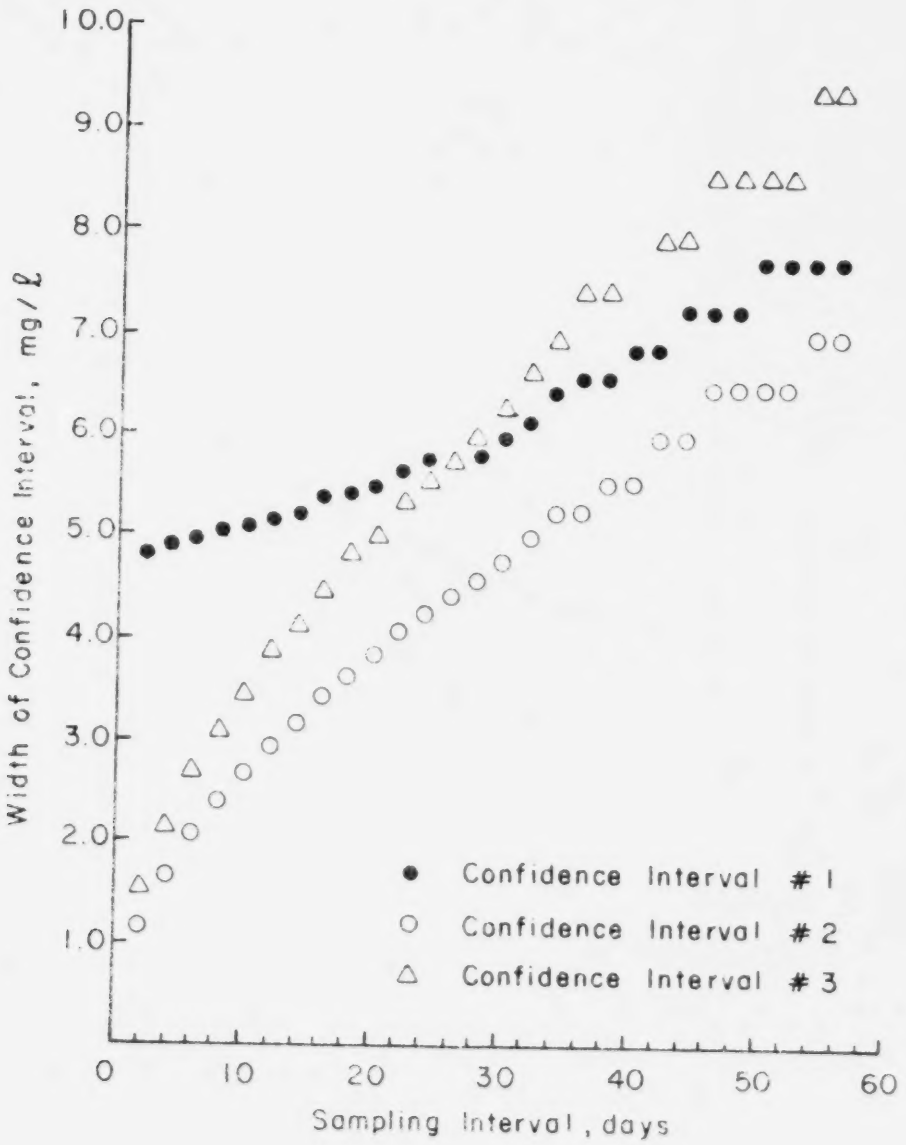

Figure 15. Average 95 percent confidence interval widths about the geometric mean for nitrates in the Illinois network.

The general behavioral pattern seen in Figure 10 is repeated here. The effect of serial correlation seems to become relatively insignificant for sampling intervals of about 20 days or greater in the total organic carbon and suspended solids series. The same thing occurs at an interval of about 30 days for total dissolved solids. However, the effect of serial correlation in the total hardness and nitrate series seems to persist out beyond sampling intervals of 40 days.

Recall that a "rule of thumb" has been suggested in the past by Ward et al. (1976) and others that samples may be considered to be independent when collected monthly or less frequently. The current analysis would indicate that this assumption is reasonably correct. It should be noted, however, that this assumption strictly applies only to data records with deterministic seasonal variation removed, the seasonal component being significant over the entire range of sampling frequencies.

The task of fitting a separate model to each constituent record at each station is certainly a formidable one. Lettenmaier (1975) has suggested that many, if not most, water quality time series might be modeled using AR(1) model. He further suggested using a parameter value of $\rho_1 = 0.85$ when insufficient data are available for estimation of ρ_1. The error involved in applying this assumption is explored in Figures 16 and 17, which compare average confidence interval widths for total dissolved solids and total hardness for the Illinois network using the fitted models with those computed using an AR(1) model with $\rho_1 = 0.85$. The widths of the "actual" confidence intervals are significantly less in each case, indicating that at least for these examples the time series tend to exhibit stronger serial correlation than that of the postulated AR(1), $\rho_1 = 0.85$ model.

In the absence of adequate data to fit a time series model of the ARMA type, the use of the first-order autoregressive model is certainly justifiable. However, confidence interval widths computed subsequent to this assumption are highly dependent on the value of the lag-one autocorrelation coefficient, ρ_1. Figure 18 shows 95 percent confidence interval widths about the annual mean (not the geometric mean) for samples exhibiting AR(1) type correlation with several values of the parameter ρ_1 and variance equal to unity. A value of $\rho_1 = 0$ of course corresponds to uncorrelated (independent) samples. These curves were obtained from equations (5) and (15). Actual confidence interval widths would be obtained by multiplying the width obtained from Figure 18 times the square root of the variance (standard deviation) of a particular time series. A significant difference in confidence interval widths exists at high sampling frequencies from the case of $\rho_1 = 0.85$ to $\rho_1 = 0.95$.

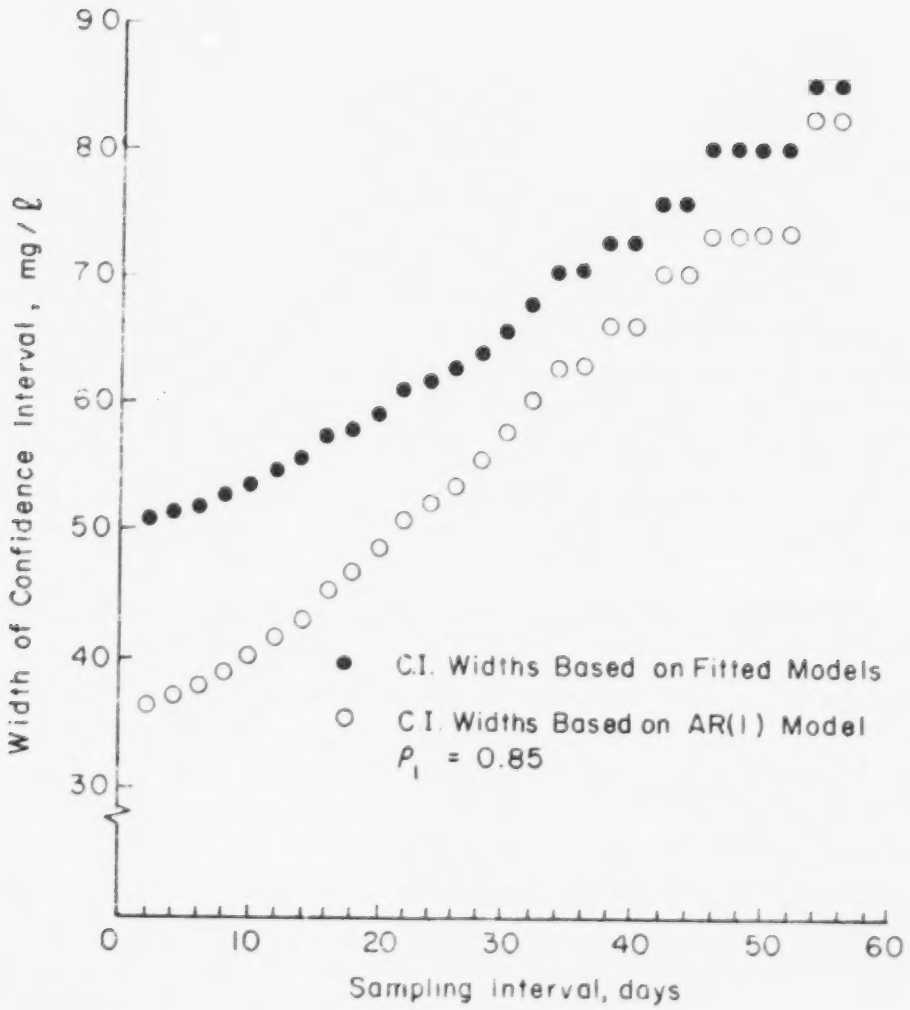

Figure 16. Average 95 percent confidence interval widths for dissolved solids concentration, Illinois network, computed from both actual fitted and hypothesized AR(1) models.

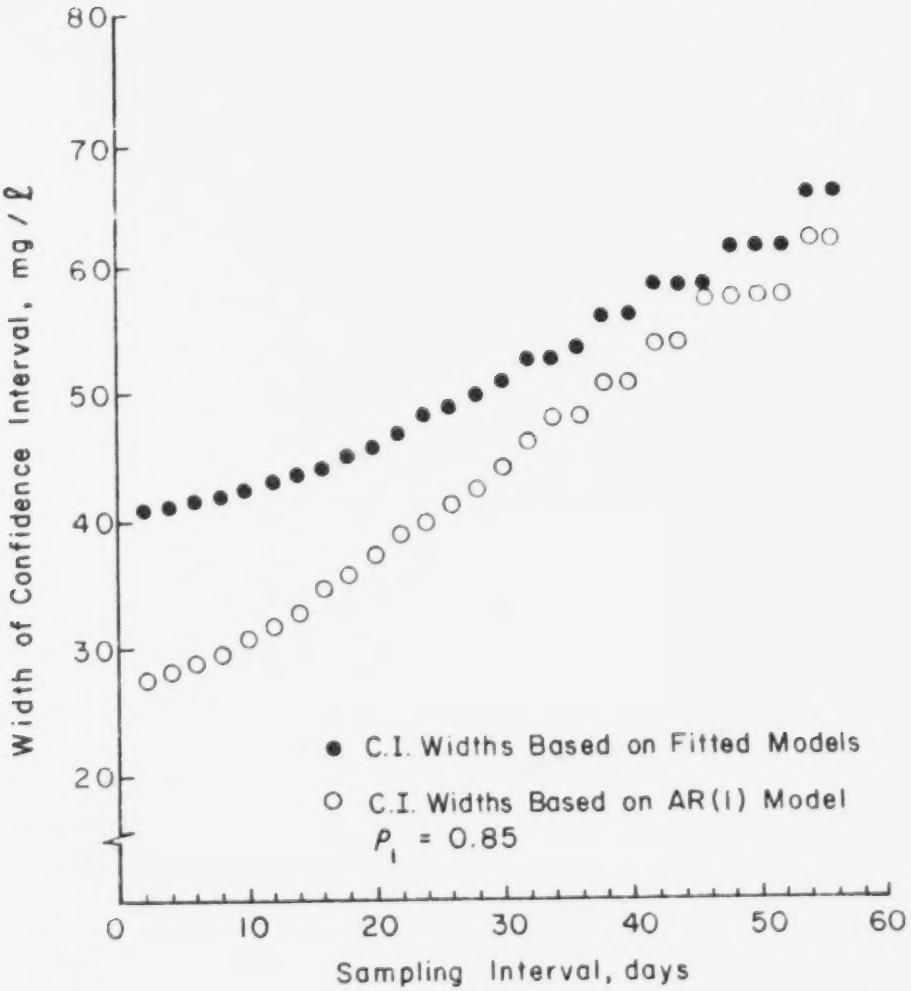

Figure 17. Average 95 percent confidence interval widths for total hardness concentration, Illinois network, computed from both actual fitted and hypothesized AR(1) models.

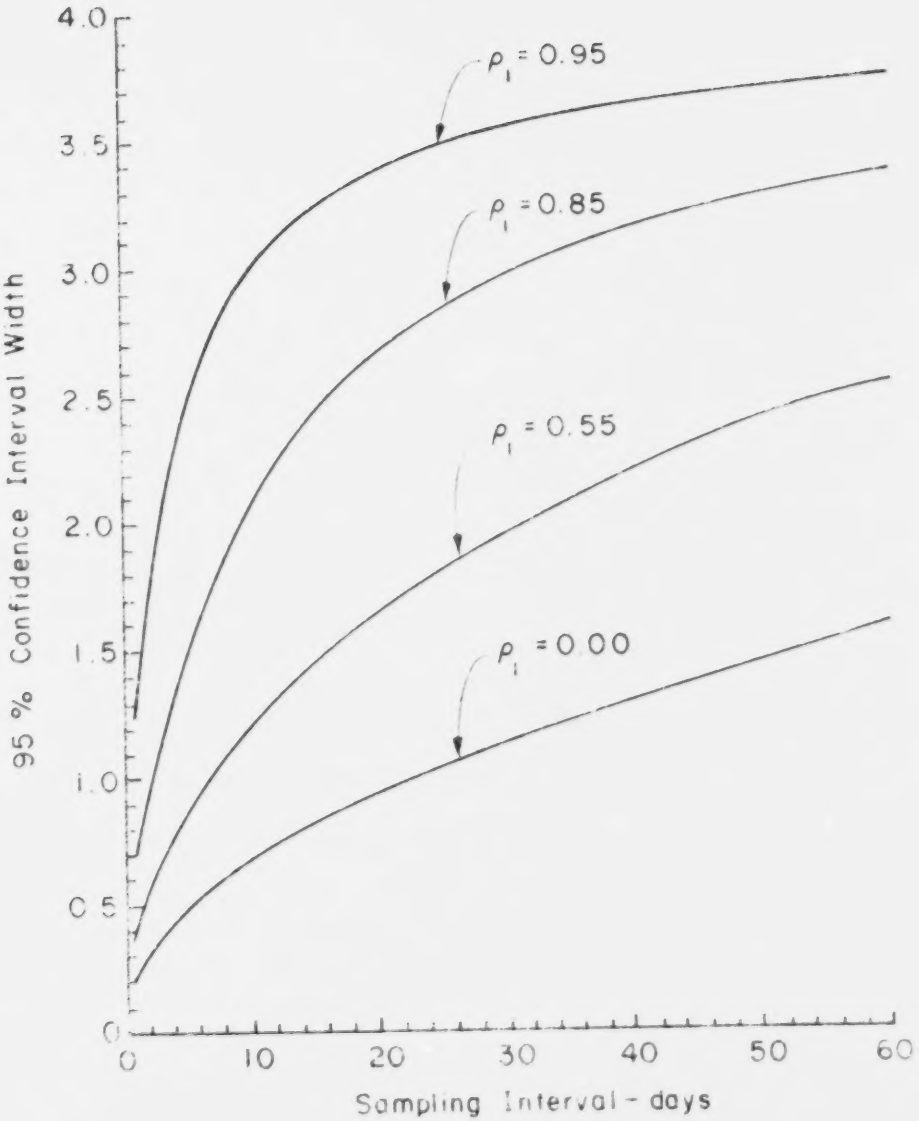

Figure 18. Effect of ρ_1 on 95 percent confidence interval widths about the annual mean for first-order autoregressive processes with unit variance.

SECTION 6

INCORPORATING ECONOMICS INTO WATER QUALITY MONITORING SYSTEM DESIGN

This section expands the application of the previously developed statistical analysis techniques to consider assigning sampling frequencies within a multistation network. Not only are confidence interval widths of several constituents considered, but also the economics of actually obtaining and analyzing the water quality sample are introduced. Given that the statistical and economic objectives are generally competing, mathematical programming is used to "optimize" the sampling frequencies.

The section is separated into three parts: (1) formulation; (2) application; and (3) sensitivity analysis. The formulation portion objectively defines the problem and establishes a dynamic programming approach to solving it. The application portion applies the dynamic programming algorithm to assigning sampling frequencies for an Illinois network for which detailed statistics are currently available. The sensitivity analysis portion evaluates the sensitivity of the sampling frequencies to changes in the design variables (e.g., changes in costs, changes in travel distances, changes in statistical design criteria, etc.).

ASSIGNING SAMPLING FREQUENCIES VIA DYNAMIC PROGRAMMING

The problem of redesigning a water quality monitoring network that is already in place may be viewed as one of assigning new sampling frequencies to each station in order to achieve improved performance. In this study the performance of a network is evaluated in terms of the confidence interval widths obtained about the annual means in quality constituents measured by the network.

The primary consideration in design is that the confidence interval widths obtained for each constituent of major concern be reasonably small and as uniform as possible from station to station. The optimization procedure presented here attempts to achieve this general objective while satisfying an economic constraint. The statistical objective of the design is to minimize the double summation--over both stations and constituents--of the positive differences between predicted confidence interval widths and design confidence interval widths for selected quality constituents. The economic constraint ensures that the sum of the operating costs over all stations will be less than the specified annual budget. The cost of sampling at each station is assumed to consist of the direct travel cost plus the laboratory cost of processing the samples.

In general the design will be based only on a small number of quality constituents that are considered to be most important by the management agency rather than on the total number of constituents actually measured. Also a limited number of possible sampling frequencies that reflect the agency's options in this area will be considered.

Problem Definition

The optimization problem may be expressed mathematically as:

$$\text{Minimize} \sum_{i=1}^{N} \sum_{j=1}^{M} \left[\frac{X_{ij} - X_j^D}{X_j^D} \right] \tag{17}$$

subject to:

$$\sum_{i=1}^{N} C_i \leq C_T \tag{18}$$

$$C_i = f_c(u_i, i) \qquad i = 1, 2, \ldots N \tag{19}$$

$$X_{ij} = f_x(u_i, j) \qquad i = 1, 2, \ldots N \quad j = 1, 2, \ldots M \tag{20}$$

$$X_j^D = \text{a constant} \qquad j = 1, 2, \ldots M \tag{21}$$

$$C_T = \text{a constant} \tag{22}$$

$$X_{ij} - X_j^D = 0 \qquad \text{if } X_{ij} - X_j^D < 0 \tag{23}$$

where X_{ij} = predicted confidence interval width for constituent j at station i

X_j^D = design confidence interval width for constituent j

C_i = annual cost of sampling at station i

C_T = total annual operating budget

u_i = number of samples collected per year at station i

N = total number of station considered

M = total number of constituents included in the design

Note that the difference $X_{ij} - X_j^D$ is set equal to zero if it would otherwise be negative since one would not normally wish to allow the objective function to benefit from a station that had achieved a confidence interval width that was smaller than that actually sought.

The differences, $X_{ij} - X_j^D$, are normalized by dividing by the design confidence interval width, X_j^D, in order that the summation can be performed over several different quality constituents whose confidence interval widths might differ greatly in magnitude.

Also note that only operating costs are considered. This arises from the assumption that the general level and extent of the monitoring operation have been established and optimization is performed within a fairly narrow region around this level. Thus fixed costs such as equipment costs and personnel salaries will remain relatively constant within the range of decisions under consideration. Another way to view the situation is that monetary resources devoted to monitoring are being reallocated in order to improve system performance. Only those resources that are actually affected by the reallocation need be included in the analysis. Since changing sampling frequencies would result in different numbers of samples to be processed and different distances to be traveled, there are the costs considered in expression (19), which for this study is assumed to be linear.

Linear Programming Approach

The functional relation (20)--and thus the objective function--is nonlinear; therefore, linear programming cannot be used to solve the problem as it stands. If the objective function were expressed as a linear function of sampling interval rather than numbers of samples collected, then expression (19) would become nonlinear and nothing is accomplished. One approach suggested by Ward et al. (1976) is to reformulate the problem as follows:

$$\text{Min} \sum_{i=1}^{N} \sum_{j=1}^{M} \left| I_{ij} - I_j^D \right| \tag{24}$$

Subject to similar constraints where I_{ij} and I_j^D are predicted and design information contents, respectively, I_{ij} is defined by

$$I_{ij} = \frac{u_i}{\sigma_{ij}^2} \tag{25}$$

where σ_{ij}^2 = variance of constituent j at station i, a known population parameter

Thus the information content is a linear function of the number of samples collected, and linear programming techniques apply. Assuming independent samples, the information content as defined above is the reciprocal

of the variance of the sample mean. It follows that achieving equal information contents would also achieve equal confidence intervals. Of course the expression for the variance of the sample mean becomes much more complicated as serial correlation becomes important as shown in equation (5).

The linear programming approach, therefore, suffers from its inability to deal with confidence interval widths directly. An additional drawback is that computed "optimal" sampling frequencies may take on fractional values unless an integer programming technique is used. An integer, linear programming formulation is also presented in Ward et al. (1976).

Dynamic Programming Approach

A mathematical programming technique that overcomes all of these difficulties and is both simple and computationally efficient is dynamic programming. This is a technique that requires no assumption of linearity in either the objective function or constraints. The discrete form of dynamic programming, which is applied here, has the further advantage that the analytical form of the objective function and constraints need not be known. Additionally, only specific values of the decision variable--i.e., specific sampling frequencies--need be considered. Thus dynamic programming can be applied as an integer technique.

The limitations of dynamic programming that relate to this application are that no "cookbook" formulation of a "typical" dynamic programming problem exists, and, therefore, one cannot normally use an off-the-shelf computer code for his particular problem as one can in the case of linear programming. However, dynamic programming codes that are specific to a particular situation are usually not as difficult to write as are other types of optimization codes.

There are also some advantages inherent in preparing one's own optimization code. The first is that a code written for a particular problem is usually more efficient than one prepared to handle all problems in a general class. A second advantage is that the writer of a code will have a better feel for its operation and therefore will be less inclined to accept erroneous results. Finally, one can gain valuable insight into the nature of the system he is dealing with as a result of the careful thinking necessary to formulate a mathematical programming code used to optimize that system. Dynamic programming was, therefore, selected as the optimization technique for this study, and a computer program was written to solve the specific problem previously described.

Summary of the Dynamic Programming Algorithm

The theory and mechanics of dynamic programming may be found in many optimization texts. A very simple presentation of the subject that is, nevertheless, adequate for most purposes is contained in Hillier and Lieberman (1974). A brief discussion will be presented here.

Dynamic programming is a technique for making a sequence of interrelated decisions. The problem is divided into stages, with a policy decision

required at each stage. Each stage has a number of states associated with it. The effect of a decision is to transform the current state into a new state at the next stage. Each decision also makes an individual contribution to the objective function. The optimization algorithm chooses the sequence of decisions that minimizes (or maximizes) the overall value of the objective function. The algorithm makes use of a recursive relation to find the optimal sequence of decisions without considering all of the possible sequences.

Given the current stage and state, the minimum value of the objective function over all succeeding stages is called the return function. The minimum value of the return function, which results from making the appropriate current decision, is known as the optimal return function. The recursive relation expresses the value of the return function for the current stage and state in terms of the contribution from making the current decision and the value of the optimal return function for the new state at the next stage that results.

Beginning at the last stage, the optimization proceeds by moving backwards, defining and storing the value of the optimal return function and the associated minimizing decisions for each possible state in each stage. When the first stage is reached, there is a single possible state known as the initial condition. Thus, the optimal return function has a single value that is the minimal value of the objective function for the overall problem. The decision that achieves this minimum is chosen as the first policy decision. Since this decision results in a unique state at the second stage, it is possible to recall the decision associated with the optimal return function for that state. This decision is chosen as the second policy decision, and so on, until all policy decisions are made.

Dynamic Programming Formulation of the Monitoring Problem

The above general concepts are applied to the water quality monitoring problem as follows.

Define:

u_i = decision variable for stage i; number of samples collected per year at station i

S_i = state variable for stage i; portion of total budget remaining

$\sum_{j=1}^{M} \frac{(X_{ij} - X_j^D)}{X_j^D}$ = contribution to objective function at stage i

$f_i(S_i, u_i)$ = return function for stage i

$f_i^*(S_i)$ = minimum u_i

$\left[f_i(S_i,u_i)\right]$ = optimal return function for stage i

i,j = subscripts referring to station and constituent, respectively

The value of the optimal return function corresponding to stage i and state S_i represents the minimum possible value of the objective function that could result from sampling at stations i through N, given that there are S_i dollars currently remaining in the budget. Thus:

$$f_i^*(S_i) = \min_{u_i}\left(\sum_{\ell=i}^{N}\sum_{j=1}^{M}\frac{X_{\ell j} - X_j^D}{X_j^D}\right) \tag{26}$$

The value of u_i that minimizes $f_i(S_i,u_i)$ is denoted as $u_i^*(S_i)$. The function $u_i^*(S_i)$ might be called an "optimal decision function" analogous to the optimal return function $f_i^*(S_i)$. Therefore:

$$f_i^*(S_i) = f_i(S_i,u_i^*) \tag{27}$$

The value of the state variable at stage i+1 may be expressed in terms of the current state and current decision as follows:

$$S_{i+1} = S_i - C_i \tag{28}$$

and:

$$C_i = f_c(u_i,i)$$

Thus the amount of money remaining in the budget is reduced by an amount equal to the annual cost of sampling station i at frequency u_i. This relation is known as the equation of state.

The recursive relation for this problem may be expressed as follows;

$$f_i(S_i,u_i) = \sum_{j=1}^{M}\frac{(X_{ij} - X_j^D)}{X_j^D} + f_{i+1}^*(S_{i+1}) \tag{29}$$

$$= \sum_{j=1}^{M}\frac{(X_{ij} - X_j^D)}{X_j^D} + f_{i+1}^*(S_i - C_i)$$

$$= \sum_{j=1}^{M}\frac{(X_{ij} - X_j^D)}{X_j^D} + \min_{u_{i+1}}\left(\sum_{\ell=i+1}^{M}\sum_{j=1}^{M}\frac{(X_{\ell,j} - X_j^D)}{X_j^D}\right) \tag{30}$$

An important point to remember is that each minimization over u_i is constrained such that S_{i+1} is always greater than or equal to zero. Thus $S_N \geq 0$, and the total budget is never exceeded.

Recalling the definition given earlier, this relation expresses the minimum value of the objective function (minimum sum of deviations from design confidence intervals) resulting from sampling at stations i through N, given a current state S_i and making the current decision u_i in terms of the contribution from the current stage:

$$\sum_{j=1}^{M} \frac{X_{ij} - X_j^D}{X_j^D}$$

and the optimal return function for the new state at the next stage, $f^*_{i+1}(S_{i+1})$.

The sequence of calculations involved in the operation of the dynamic programming code is illustrated in the flow diagram of Figure 19. As previously discussed, the general procedure is first to move backwards through the stages computing optimal return functions and optimal decision functions for each stage. The second step is, beginning with the initial condition (total budget) at the first stage, to go back through the stages, computing the new state at each stage based on the previous decision and recalling the optimal policy decision associated with each new state until the last stage is reached and the overall optimal operating policy has been attained.

The first segment of the program is composed of statistical subroutines that compute confidence intervals for each water quality constituent at each station over the range of sampling frequencies of interest. The method of computation is described in Section 5. Theoretical autocorrelation functions for adopted ARMA models are used to account for serial correlation in the time series. The required inputs for this portion include the numerical values of the ARMA model parameters for each constituent of each station and the variance of each series with deterministic seasonal variation removed.

The main portion of the program is the optimization algorithm itself, which utilizes the computed confidence intervals from the first segment in the computation of the objective function. The cost of sampling, which is used in the equation of state, is computed in a separate subroutine; this facilitates using any desired cost relations. For this research, the cost of collecting and processing a sample is considered to be the sum of the incremental cost of travel plus direct laboratory analysis costs. Thus:

$$\begin{array}{l}\text{Total annual} \\ \text{cost for} \\ \text{station}\end{array} = \begin{array}{c}\text{No. of} \\ \text{samples} \\ \text{per year}\end{array} \left[\begin{array}{c}\text{Lab cost} \\ \text{per} \\ \text{sample}\end{array} + \left(\begin{array}{c}\text{Incremental} \\ \text{travel} \\ \text{cost}\end{array} \right) \left(\begin{array}{c}\text{Incremental} \\ \text{distance} \\ \text{to station}\end{array} \right) \right] \qquad (31)$$

As mentioned previously, since only direct costs are considered in the analysis, the optimization should be regarded as an efficient reallocation

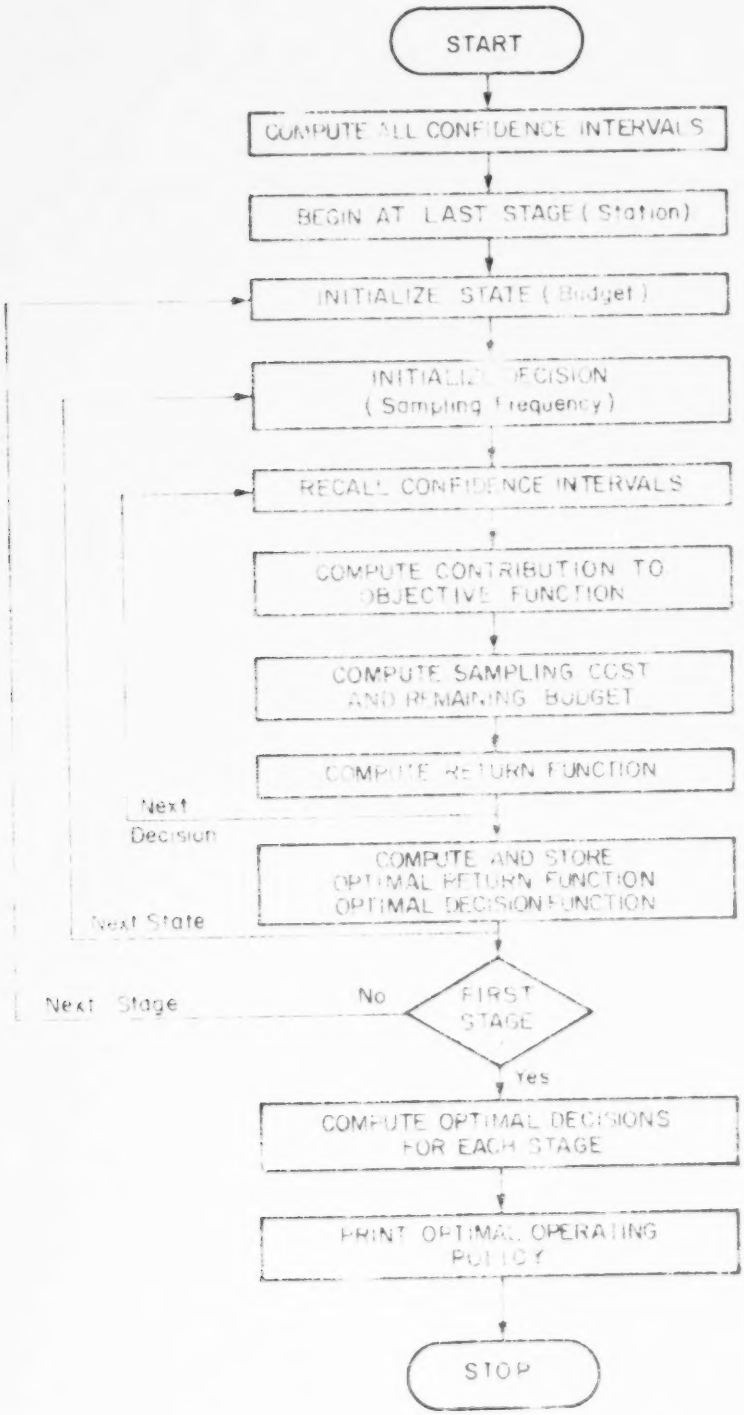

Figure 19. Flow diagram of dynamic programming code.

resources within a predetermined operating range, not as a "global" optimization of the system.

APPLICATION TO ILLINOIS NETWORK

As an illustration of the dynamic programming formulation described earlier, the network design procedure was applied to nine stations of the Illinois network for which time series models had been determined. The input factors that must be determined in order to use this approach are the following: (1) water quality constituents to be included in the design; (2) the parameters of the ARMA models used, including autoregressive constants and moving-average constants and variances; (3) design confidence interval widths; (4) incremental travel costs; (5) incremental distances for each station; (6) laboratory analyses costs; (7) total annual operating budget; and (8) sampling frequencies considered. The design values of the input variables related to the above factors were selected as follows.

Constituents Included In Design

The type and number of water quality constituents to be included in the analysis is highly subjective. The most important considerations are probably: (1) to include those constituents that can serve as indicators of the major types of quality problems (pollution) expected; and (2) to avoid including too many constituents in the design, which would result in a less effective determination of means for major indicators. For the initial or "baseline" run, five constituents were included:

1. Total dissolved solids (mg/ℓ) as an indicator of overall water quality and nonpoint-source pollution.

2. Total organic carbon (mg/ℓ) as an indicator of organic (municipal and industrial) pollution.

3. Suspended solids (mg/ℓ) as an indicator of pollution from agriculture, land clearing, and development.

4. Total hardness (mg/ℓ as calcium carbonate) as an indicator of metal ion concentration.

5. Nitrate (mg/ℓ) as a nutrient indicator.

ARMA Models

The model used in the design was the selected "best" model of the three candidates--AR(1), AR(2), and ARMA(1,1)--for each constituent at each station as listed in Table 4. Since five parameters at nine stations were used, the baseline run used 45 different models in computing confidence intervals.

Design Confidence Interval Widths

In order to assign design confidence interval widths to each constituent, a hypothetical situation was constructed in which the State agency had

sufficient resources to sample all stations uniformly at a frequency of 26 samples per year. It was desired to reassign sampling frequencies in order to achieve greater uniformity of confidence intervals. Therefore, confidence interval widths were computed for each constituent at each station based on a frequency of 26 samples per year, and the median width over all the stations was selected for this demonstration as the design value for each constituent. Other desirable criteria could be established for selecting the design value. Thus, at the uniform frequency half of the stations would be achieving the design confidence interval width and the program would reallocate samples in order to improve upon this performance. The range of and median confidence interval widths for the design constituents are presented in Table 7.

TABLE 7. MEDIAN AND RANGE OF CONFIDENCE INTERVAL WIDTHS FOR WATER QUALITY CONSTITUENTS, ILLINOIS NETWORK (95% Confidence Level, 26 Samples per Year)

Quality Constituent	Mean Confidence Interval Width	Range
Total dissolved solids (mg/ℓ)	37.0	17.0 - 132.1
Total organic carbon (mg/ℓ)	2.29	1.26 - 3.80
Suspended solids (mg/ℓ)	14.9	3.6 - 39.5
Total hardness (mg/ℓ)	36.8	23.0 - 93.1
Nitrates (mg/ℓ)	1.99	0.52 - 19.5

Incremental Travel Costs

The Illinois State Water Survey (Harmeson, 1978) indicated a direct travel cost of $0.14 per km for sampling the network used in this study. This figure should be representative of the change in travel costs an agency would experience as a result of relatively small changes in total distance traveled and would apply for the type of reallocation in sampling discussed here. This is the cost that applies in equation 31.

Laboratory Analysis Costs

The laboratory cost per sample is highly variable, depending on the type and number of constituents measured and on whether the analysis is done within the agency or contracted to an outside laboratory. The costs used in this study were based on information obtained from the Colorado State Department of Health, Water Quality Control Division. This agency routinely measures at least 35 chemical constituents (Table 8). Also given are the average costs of analysis for each constituent as reported by the U. S. Army Corps of Engineers (1978) for several independent laboratories. These costs would more nearly reflect average total costs of analysis. The State of

TABLE 8. LABORATORY ANALYSIS COSTS FOR CHEMICAL CONSTITUENTS OF WATER QUALITY

Water Quality Constituent	Laboratory Analysis Costs	
	State of Colorado*	Independent Laboratories†
1 Turbidity	0.53	3.89
2 Conductivity	0.27	3.95
3 Dissolved oxygen	2.50	4.60
4 Biochemical oxygen demand	9.96	27.19
5 Chemical oxygen demand	9.96	14.38
6 pH	0.83	3.05
7 Total volatile solids	3.00	6.63
8 Total dissolved solids	2.00	7.23
9 Total solids	2.00	7.00
10 Ammonia nitrogen	1.66	11.81
11 Nitrite nitrogen	1.66	7.50
12 Nitrate nitrogen	1.66	8.17
13 Total phosphate	1.66	5.57
14 Cyanide	4.98	19.93
15 Total hardness	1.66	4.85
16 Calcium	1.66	7.56
17 Magnesium	0.50	8.56
18 Sodium	1.66	8.95
19 Chloride	1.33	5.79
20 Sulfate	2.67	8.75
21 Fluoride	0.83	12.00
22 Arsenic	9.96	16.29
23 Boron	1.66	10.42
24 Cadmium	4.98	7.56
25 Chromium	4.98	9.05
26 Copper	4.98	7.88
27 Iron	1.66	8.24
28 Lead	4.98	10.47
29 Manganese	1.66	19.20
30 Silver	1.66	10.70
31 Zinc	1.66	9.63
32 Mercury	7.47	17.50
33 Kjeldahl nitrogen	9.96	18.05
34 Aluminum	1.66	10.96
35 Potassium	1.66	8.77
Total	111.91	342.08

*From Anderson, 1978.

†From U.S. Army Corps of Engineers, 1978.

Colorado performs its own laboratory analyses and reports an average cost of $111.91 per sample (Anderson, 1978). This cost is taken to represent operating costs of the laboratory excluding overhead. Since this study deals with changes in operating costs, a per-sample cost of $110 was used in the network design. Note that if some samples were analyzed for fewer than the total number of constituents, a smaller laboratory cost would apply. A more complex economic analysis would be necessary, however, if the assumption that all samples are processed identically were removed.

Determining Incremental Distances

The cost of collecting additional samples at a particular station is more nearly a function of the "remoteness" of that station from other stations in the network than it is of the actual distance from that station to the laboratory. This is true of course since the sampling unit normally travels from station to station rather than from station to laboratory each time. An exact determination of travel costs would require a consideration of the exact collection routes and would be an enormously complex task. A simpler procedure, which was adopted for this study, was to use the average one-way travel distance (approximated by a straight line) from the three stations nearest the one in question. This represents the average additional distance traveled to collect an additional sample at the station and is the distance used in equation 31. Design distances for each station in the network are presented in Table 9.

Total Budget

The design budget is the portion of the total monitoring budget that represents the direct operating cost associated with travel of the sampling units and laboratory analysis of samples. The design budget used in this study is based on the same hypothetical situation described earlier. It is assumed that the agency's total budget allows it to sample each station with a uniform frequency of 26 samples per year. The portion of that budget that is direct operating expense was calculated as follows.

The direct travel budget is the incremental travel cost (per km) times the sum over all stations of the distances associated with each station times the number of samples per year. The annual laboratory budget is the cost of processing a sample times the number of stations times the number of samples per year. The total annual operating budget is, of course, the sum of the travel and laboratory budgets. Using the baseline costs of $0.14 per km for travel, $110 per sample for laboratory analysis, and 26 samples per year, a design budget of $28,050 was obtained.

Sampling Frequencies Considered

The choice of sampling frequencies to consider is another highly subjective aspect of the design process. One approach would be to consider every integer sampling frequency between one sample per year and 365 samples per year. However, most State agencies are constrained (or feel that they are) to certain "standard" sampling frequencies--e.g., weekly, monthly, etc. The

TABLE 9. RESULTS OF DYNAMIC PROGRAMMING DESIGN OF SAMPLING FREQUENCIES FOR ILLINOIS NETWORK

(A) Individual Results

Station Number	Distance (km)	Frequency Samples/Year	Water Quality Constituent	95% Confidence Interval Widths		
				Design (mg/ℓ)	Uniform Frequency (mg/ℓ)	Predicted (mg/ℓ)
1	58.9	52	TDS	37.0	87.2	78.1
			TOC	2.29	3.80	3.14
			Suspended solids	14.9	39.5	35.2
			Hardness	36.3	64.5	57.9
			Nitrate	1.99	1.99	1.87
2	69.1	26	TDS	37.0	17.0	17.0
			TOC	2.29	2.30	2.30
			Suspended solids	14.9	12.0	12.0
			Hardness	36.3	25.1	25.10
			Nitrate	1.99	5.03	5.03
3	44.3	26	TDS	37.0	35.3	35.3
			TOC	2.29	2.38	2.38
			Suspended solids	14.9	17.8	17.8
			Hardness	36.3	36.8	36.8
			Nitrate	1.99	5.39	5.39
4	54.1	39	TDS	37.0	67.6	64.3
			TOC	2.29	2.22	1.81
			Suspended solids	14.9	14.9	12.2
			Hardness	36.3	23.0	22.1
			Nitrate	1.99	2.77	2.24
5	63.5	26	TDS	37.0	37.0	37.0
			TOC	2.29	1.92	1.92
			Suspended solids	14.9	14.3	14.3
			Hardness	36.3	36.4	36.4
			Nitrate	1.99	4.14	4.14

(continued)

TABLE 9. (continued)

Station Number	Distance (km)	Frequency Samples/Year	Water Quality Constituents	95% Confidence Interval Widths		
				Design (mg/ℓ)	Uniform Frequency (mg/ℓ)	Predicted (mg/ℓ)
6	67.2	26	TDS	37.0	132.1	132.1
			TOC	2.29	2.29	2.29
			Suspended solids	14.9	23.6	23.6
			Hardness	36.3	93.1	93.1
			Nitrate	1.99	19.5	19.5
7	79.2	13	TDS	37.0	58.8	60.0
			TOC	2.29	2.40	2.82
			Suspended solids	14.9	5.40	7.18
			Hardness	36.3	39.3	40.3
			Nitrate	1.99	1.49	2.01
8	119.7	13	TDS	37.0	28.8	32.8
			TOC	2.29	1.65	2.30
			Suspended solids	14.9	6.90	9.17
			Hardness	36.3	31.9	35.1
			Nitrate	1.99	4.95	5.37
9	98.5	13	TDS	37.0	33.3	33.7
			TOC	2.29	1.26	1.41
			Suspended solids	14.9	4.54	5.50
			Hardness	36.3	41.1	41.2
			Nitrate	1.99	1.62	1.67

(continued)

TABLE 9. (continued)

(B) Summary Statistics

Constituent		Uniform Frequency Sampling (mg/ℓ)	Predicted (mg/ℓ)	% Change
TDS	Mean =	55.3	54.5	- 1.5
	Standard deviation =	35.2	34.8	- 1.1
TOC	Mean =	2.25	2.26	+ 0.4
	Standard deviation =	0.70	0.52	-25.8
Suspended solids	Mean =	15.4	15.2	- 1.3
	Standard deviation =	10.9	9.3	-14.7
Total hardness	Mean =	43.5	43.1	- 0.9
	Standard deviation =	22.0	21.3	- 3.2
Nitrate	Mean =	5.21	5.25	+ 0.7
	Standard deviation =	5.57	5.57	0.0

Average % change in mean confidence interval widths = -0.5

Average % change in standard deviation of confidence interval widths = -10.3

dangers of considering only such frequencies are discussed elsewhere, such as in Sanders (1974). Briefly, the problem is that of sampling at the same point in every cycle of an underlying cyclic variation in quality. For example, sampling on the same day in every week in a stream that exhibits a weekly cycle in flow will cause aliasing of the collected water quality data. A study of underlying cyclic variations in quality is, therefore, essential before the selection of candidate sampling frequencies is made. A mathematical tool for performing such a study is spectral analysis. The application of this tool to water quality is described in Wastler (1963).

Nevertheless, for this study, "standard" sampling frequencies ranging from twice a week to every two months were considered. Specifically, the possible frequencies were 104, 52, 39, 26, 13, and 6 samples per year.

Results

The results of the design procedure may be found in Table 9. The table shows the computed design sampling frequencies, design confidence interval widths for each quality constituent, confidence interval widths that would result from a uniform frequency of 26 samples per year at all stations, and confidence interval widths that would result from the design sampling frequency.

The level of improvement afforded by design sampling frequencies over uniform sampling frequencies may be examined by comparing the means and standard deviations of the confidence interval widths obtained in each case. These results are also included in the table.

Taking an average over all five constituents, the mean confidence interval widths decreased by 0.5 percent with respect to a uniform frequency program, and the standard deviation of the confidence interval widths decreased by 10.3 percent. Although using the same resources as uniform sampling and allocating them via dynamic programming did not greatly improve the average-size confidence intervals, it did provide for 10.3 percent more uniformity in confidence widths across the network.

SENSITIVITY ANALYSIS

In order to determine how sensitive the dynamic programming solution is to changes in the values of the input variables, the design problem was repeated several times with a variety of input conditions. The results were compared using the solution obtained previously as the standard of comparison (or baseline run).

Incremental Travel Costs

The operating cost of travel was varied from \$0.00 to \$0.50 per km with a baseline cost of \$0.14 per km. Costs of \$0.00, \$0.10, \$0.14, \$0.18, \$0.22, and \$0.26 per km yielded the same solution. However a cost of \$0.50 per km produced an increase in number of samples at station #3, which has a distance of 44.3 km, and a decrease at station #9, which has a distance of 88.5 km. These results are presented in Table 10. The lack of sensitivity to travel

cost is expected since, for this example, the travel cost represents a rather small fraction of the total design budget as indicated in the table.

TABLE 10. DESIGN SAMPLING FREQUENCIES BASED ON VARYING TRAVEL COSTS

Station	Distance (km)	Design Frequency (samples/yr) for Cost = $0.14/km	Design Frequency (samples/yr) for Cost = $0.50/km
1	58.9	52	52
2	69.1	26	26
3	44.3	26	39
4	54.1	39	39
5	63.5	26	26
6	67.2	26	26
7	79.2	13	13
8	119.7	13	13
9	88.5	13	6
Total distance	644.5		
Annual travel cost		2,350	8,350
Lab analysis cost		25,750	25,750
Total annual cost		$28,100	$34,100

Distances to Each Station

An alternate method of determining the distance associated with each station was evaluated by using the one-way travel distance from the laboratory to the station. For these alternate distances, travel costs of $0.14 and $0.50 per km were applied. The results in the case of $0.14 per km are the same as the baseline results except the alternate mileages produce a sampling frequency of 6 samples per year rather than 13 at station #9. In the case of $0.50 per km, there is additionally a shift of six samples per year from station #1, which has a distance of 160 km, to station #7 which has a distance of 120 km. These results are presented in Table 11.

Annual Operating Budget

The economic reasoning behind this study should apply for small variations about some predetermined level of activity. A variation of less than $\pm$ 10 percent in the total budget was investigated while maintaining the baseline travel and laboratory analysis costs. As indicated in Table 12 a considerable difference in solutions resulted. The $2,600 decrease in budget resulted in a design total of fewer samples collected per year while the

$2,600 increase resulted in a total of 19 more samples per year than in the baseline run.

TABLE 11. DESIGN SAMPLING FREQUENCIES BASED ON ALTERNATE TRAVEL DISTANCES

Station	Distance (km)	Design Frequency (samples/yr) for cost = $0.14/km	Design Frequency (samples/yr) for Cost = $0.50/km
1	160	52	39
2	122	26	26
3	150	26	26
4	174	39	39
5	158	26	26
6	98	26	26
7	120	13	26
8	168	13	13
9	78	6	6
Total distance	1,228		
Annual travel cost		4,500	15,950
Lab analysis cost		25,750	25,750
Total annual cost		$30,250	$41,700

The means and standard deviations of confidence interval widths for each constituent are also given in Table 12 at each of the three budget levels.

At the lower budget ($25,500), the mean confidence interval width increased by an average of 1.1 percent compared to a uniform frequency program while the average standard deviation of the confidence interval widths decreased by 9.6 percent. At the higher budget ($30,700) the mean confidence interval width decreased by 1.2 percent, and the average standard deviation of the confidence interval widths decreased by 12.7 percent when compared to the uniform frequency program. In retrospect, the baseline budget of $28,100 produced decreases in the average means and average standard deviations of confidence interval widths of 0.5 percent and 10.3 percent, respectively. Note that the changes in the mean confidence interval widths are insignificant in all cases, but improvements in uniformity of confidence intervals are important.

Design Confidence Interval Widths

The design confidence interval widths for each constituent were reassigned based on a uniform sampling frequency of 13 samples per year. The total budget was accordingly reduced from $28,100 to $14,050. The alternate design

TABLE 12. EFFECT OF VARIATION IN TOTAL OPERATING BUDGET ON DESIGN SAMPLING FREQUENCIES AND MONITORING SYSTEM PERFORMANCE, ILLINOIS NETWORK

(A) $25,500 Budget		Predicted Confidence Interval Widths				
Station Number	Design Sampling Frequency (samples/year)	TDS (mg/ℓ)	TOC (mg/ℓ)	SS (mg/ℓ)	Hardness (mg/ℓ)	NO_3^- (mg/ℓ)
1	39	80.7	3.32	36.4	59.8	1.91
2	26	17.0	2.30	12.0	25.10	5.03
3	26	35.3	2.38	17.8	36.8	5.39
4	39	64.3	1.81	12.2	22.1	2.24
5	26	37.0	1.92	14.3	36.4	4.14
6	26	132.1	2.29	23.6	93.1	19.5
7	13	60.0	2.82	7.2	40.3	2.01
8	13	32.8	2.30	9.2	35.1	5.37
9	6	35.8	1.86	8.1	42.2	1.88
Total samples	214					
Mean confidence interval width		55.0	2.33	15.6	43.4	5.27
% change over uniform frequency		-0.5	+3.5	+1.3	-0.2	+1.2
Standard deviation of confidence interval widths		34.9	0.49	9.3	21.5	5.55
% change over uniform frequency		-0.9	-30.3	-14.4	-2.3	-0.3

Average % change in mean confidence interval width = 1.1

Average % change in standard deviation of confidence interval widths - 9.6

(continued)

TABLE 12. (continued)

(B) $30,700 Budget		Predicted Confidence Interval Widths				
Station Number	Design Sampling Frequency (samples/year)	TDS (mg/ℓ)	TOC (mg/ℓ)	SS (mg/ℓ)	Hardness (mg/ℓ)	NO_3^- (mg/ℓ)
1	52	78.1	3.14	35.2	57.9	1.87
2	26	17.0	2.30	12.0	25.10	5.03
3	39	31.4	2.15	16.7	35.4	5.11
4	39	64.3	1.81	12.2	22.1	2.24
5	26	37.0	1.92	14.3	36.4	4.14
6	26	132.1	2.29	23.6	93.1	19.50
7	26	58.8	2.40	5.4	39.3	1.49
8	13	32.8	2.30	9.2	35.1	5.37
9	6	35.8	1.86	8.1	42.2	1.88
Total samples	253					
Mean confidence interval width		54.1	2.24	15.2	42.9	5.18
% change over uniform frequency		-2.2	-0.4	-1.3	-1.4	-0.5
Standard deviation of confidence interval widths		34.9	0.40	9.2	21.4	5.59
% change over uniform frequency		-2.0	-42.6	-15.7	-2.7	+0.3

Average % change in mean confidence interval width = -1.2

Average % change in standard deviation of confidence interval widths = -12.7

confidence interval widths and resulting sampling frequencies are shown in Table 13. These results represent a reallocation of samples about a uniform frequency of 13 samples per year rather than 26 samples per year as in previous designs, but the same stations tend to get the greatest number of samples as in the baseline run.

TABLE 13. EFFECT OF DESIGN CONFIDENCE INTERVAL WIDTHS ON DESIGN SAMPLING FREQUENCIES

Constituent	(a) Design Confidence Interval Widths Based on 26 Samples/Year, (mg/ℓ)	(b) Design Confidence Interval Widths Based on 26 Samples/Year, (mg/ℓ)
Total dissolved solids	37.0	47.4
Total organic carbon	2.29	2.82
Suspended solids	14.9	19.7
Total hardness	36.8	40.3
Nitrates	1.99	5.10
Station	**Sampling Frequency (samples/year)**	**Sampling Frequency (samples/year)**
1	52	26
2	26	13
3	26	13
4	39	13
5	26	13
6	26	13
7	13	6
8	13	13
9	13	6
Total samples	234	116

Water Quality Constituents Included

Sampling frequencies were determined based on a single constituent (total dissolved solids) and on three constituents (total dissolved solids, total organic carbon, and nitrates), in addition to the baseline run with five constituents. The results are presented in Table 14 using the same summary statistics as before. As one would expect, the greatest improvement for the design constituents is seen when fewer are included in the design.

Since the concentrations of many water quality constituents are quite correlated with each other (or to flow), one would expect an improvement in overall uniformity of confidence interval widths from designs based on only a

TABLE 14. EFFECT OF WATER QUALITY CONSTITUENT SELECTION ON DESIGN SAMPLING FREQUENCIES AND SYSTEM PERFORMANCE, ILLINOIS NETWORK

(A) Design Based on TDS Only

Station Number	Design Sampling Frequency (samples/year)	Predicted Confidence Interval Widths				
		TDS (mg/ℓ)	TOC (mg/ℓ)	SS (mg/ℓ)	Hardness (mg/ℓ)	NO_3^- (mg/ℓ)
1	52	78.1	3.14	35.2	57.9	1.87
2	6	33.0	4.00	17.8	47.4	7.57
3	26	35.3	2.38	17.8	36.8	5.39
4	52	62.8	1.54	10.9	21.7	1.99
5	26	37.0	1.92	14.3	36.4	4.14
6	26	132.1	2.29	23.6	93.1	19.50
7	26	58.8	2.40	5.4	39.3	1.49
8	13	32.8	2.30	9.2	35.1	5.37
9	6	35.8	1.86	8.1	42.2	1.88
Total samples	233					
Mean confidence interval width		56.2	2.43	15.8	45.5	5.47
% change over uniform frequency		-1.6	+8.0	+2.6	+4.5	+5.0
Standard deviation of confidence interval widths		32.8	0.740	9.2	20.3	5.67
% change over uniform frequency		-6.8	+6.0	-15.6	-7.8	+1.8

Average % change in mean confidence interval width = +3.7

Average % change in standard deviation of confidence interval widths = -4.5

(continued)

TABLE 14. (continued)

(B) Design Based on TDS, TOC, and NO_3^-

Station Number	Design Sampling Frequency (samples/year)	TDS (mg/ℓ)	TOC (mg/ℓ)	SS (mg/ℓ)	Hardness (mg/ℓ)	NO_3^- (mg/ℓ)
1	39	80.7	3.32	36.4	59.8	1.91
2	26	17.0	2.30	12.0	25.10	5.03
3	26	35.3	2.38	17.8	36.8	5.39
4	39	64.3	1.81	12.2	22.1	2.24
5	26	37.0	1.92	14.3	36.4	4.14
6	26	132.1	2.29	23.6	93.1	19.50
7	26	58.8	2.40	5.4	39.3	1.49
8	13	32.8	2.30	9.2	35.1	5.37
9	6	35.8	1.86	8.1	42.2	1.88
Total samples	227					
Mean confidence interval width		54.9	2.29	15.4	43.3	5.22
% change over uniform frequency		-0.7	+1.8	0.0	-0.5	+0.2
Standard deviation of confidence interval widths		34.9	0.46	9.5	21.5	5.59
% change over uniform frequency		-0.8	-34.1	-12.8	-2.3	+0.4

Average % change in mean confidence interval widths = +1.6

Average % change in standard deviation of confidence interval widths = -9.9

very few constituents. These results support that conclusion. Also, as more constituents are included, the individual improvements become compromised and less and less is gained. One could conclude that if each of the 30 measured constituents were equally important, uniform frequency sampling would be the best alternative.

SECTION 7

SYNOPSIS

Three sets of data records for several water quality constituents were analyzed to examine the effects of using various levels of statistics to design water quality monitoring networks. The effects measured were the errors in computing confidence interval widths about the annual mean for each constituent.

For each set of data, an estimate of the deterministic annual variation and serial correlation structure was computed. The annual cycles were determined by estimating the coefficients A and C of the equation:

$$y_t = A(\cos wt + C) \tag{32}$$

where y_t = deterministic component at time t

w = 360 degrees/number of samples per year

The correlation structures were determined by fitting the coefficients, ϕ_1, ϕ_2, and θ_1, of the autoregressive, moving-average model:

$$Z_t = d_1 Z_{t-1} + d_2 Z_{t-2} + a_t - R_1 a_{t-1} \tag{33}$$

where Z_t = value of time series at time t

a_t = random noise at time t

for each water quality constituent and then calculating theoretical autocorrelation functions based on the fitted models.

Confidence interval widths about annual geometric means were then determined for a range of sampling frequencies for each constituent. The confidence interval widths were computed in three ways:

1. Based on the variance of the correlated noise (σ_z^2) and accounting for the effect of serial correlation.

2. Based on the variance of the series with the deterministic component removed (variance of correlated noise).

3. Based on the variance of the original time series.

The relative error resulting from using the simpler computational methods, the second and third as compared with the first method was examined.

A dynamic programming code was then formulated for the purpose of assigning sampling frequencies throughout a network in order to minimize a statistical objective function with an economic constraint. The objective function is the sum (over several selected constituents and all stations) of the normalized positive deviation of the predicted confidence interval widths from preselected design confidence interval widths. The code was designed to account for the effects of deterministic seasonal variation and serial correlation by incorporating the results of the time series analysis just described. The economic constraint ensures that the annual operating cost of the system, including direct costs of travel and laboratory analysis, will not exceed the allowable budget.

As an example situation, the dynamic programming code was used to assign sampling frequencies to the nine stations in Illinois from which data had been obtained and analyzed. Design confidence interval widths were adopted as the median confidence interval width for each constituent over all stations based on a sampling frequency of 26 samples per year. Using five design water quality constituents and representative travel and laboratory costs, a baseline design was produced. A sensitivity analysis was then performed by varying the values of the input parameters of the optimization routine. The input variables that were varied included the cost of travel, annual operating budget, design confidence interval widths, and number of quality constituents included in the analysis.

SECTION 8

ASSUMPTIONS

Water quality monitoring involves sampling a correlated time series, which is a realization of a stochastic process, the exact nature of which is unknown. Thus assumptions have to be made relative to the way in which a water quality population varies over time. Additional assumptions are necessary in order to facilitate an economic analysis. Consequently, the results of this research should be viewed in light of the limitations under which the research was conducted.

Perhaps the most serious limitation is the lack of adequate historical water quality records. The records used in this study are among the best available today, and yet their limited length is inadequate for an accurate estimation of deterministic seasonal components and somewhat inadequate for fitting time series models. Practically speaking, regulatory agencies will seldom have daily water quality records. However, records consisting of infrequent and unevenly spaced observations may be used to estimate deterministic seasonal cycles provided the record length is adequate. A closely related limitation is the assumption that estimated population parameters such as the mean and variance represent true population values. Such an assumption is, of course, only as good as the data used in estimation.

Although this report deals strictly with sampling frequency selection, it is essential that sample collection procedures be evaluated and improved as a part of any upgrading of a water quality monitoring system. This improvement should be geared toward assuring that future samples are representative in both space and time of water quality conditions as they actually exist in the stream.

Some common problems in sample collection that produce distorted water quality information are failure to account for weekly cyclic variation in quality, failure to account for diurnal variation in quality, and failure to account for cross-sectional variation in quality. Some possible solutions to these problems are: (1) using sampling intervals other than multiples of a week; (2) collecting 24-hour composite samples; and (3) collecting multiple samples along each stream cross section, respectively. A more in-depth discussion of these considerations is presented in Sanders (1974).

A major limitation with regard to the application of these results is that of statistical and mathematical expertise required by agency personnel. Virtually all of the techniques described here would require some additional training of personnel. However, all of them can be applied in "cookbook" fashion without an understanding of all of the underlying mathematics.

Fitting ARMA models requires that the necessary software packages (such as IMSL) be available, but the other procedures--fitting the seasonal component, computing confidence interval widths, and assigning sampling frequencies via dynamic programming--can be accomplished if well-documented Fortran programs are supplied to agencies.

A third limitation is that imposed by the economic viewpoint taken here. This viewpoint requires that an existing network be in operation, that the overall scale of the monitoring network not be subject to change, that the fraction of the total budget allocated to operating costs of travel and laboratory analysis be identified, and that incremental costs resulting from a reallocation of sampling frequencies be identified. This viewpoint is admittedly restrictive, but in order to extend the analysis to optimize the total monitoring program in an economic sense, it would be necessary to translate the value of water quality data into dollars and cents. Such an objective would require an extensive research effort beyond that attempted here.

A final limitation on the value of these results is caused by the failure of most regulatory agencies to carefully define the ultimate use of water quality data in management decisions. Without such definition there cannot exist fully rational approaches toward the more subjective aspects of network design. In the design procedures outlined here, the subjective aspects include the selection of water quality constituents to be included in the analysis and the assignment of design confidence interval widths for each constituent.

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APPENDIX

ESTIMATED VALUES OF DETERMINISTIC COEFFICIENTS FOR SEASONAL COMPONENTS OF WATER QUALITY TIME SERIES

Location	Water Quality Constituent log (mg/ℓ)	$y_t = A \cos(wt + C) + mt$ A	C	m
Grand River, Michigan	Specific conductance (μmhos/cm)	-0.105	1.03	0.446
	Total phosphate	-0.171	1.23	0.0013
	Sulfate	-0.119	0.462	0.0816
	Chloride	-0.334	0.718	0.0015
Red River, Manitoba	Specific conductance (μmhos/cm)	0.265	1.94	
	Bicarbonate	0.276	65.4	
	Sodium	0.508	1.37	
	Chloride	0.653	1.47	
Little Wabash River, Illinois, Sta. 1	TDS	-0.268	5.60	
	TOC	0.0646	-0.0771	
	SS	-1.15	1.46	
	Hardness	0.344	8.81	
	Nitrate	0.369	1.54	
Kankakee River, Illinois, Sta. 2	TDS	0.0410	1.21	
	TOC	-0.357	1.80	
	SS	-1.47	1.72	
	Hardness	-0.0301	0.997	
	Nitrate	-.394	0.790	

(continued)

APPENDIX (continued)

Location	Water Quality Constituent log (mg/ℓ)	y_t = A cos (wt + C) + mt A	C	m
Kankakee River, Illinois, Sta. 3	TDS	0.0648	1.14	
	TOC	-0.282	1.84	
	SS	-1.35	1.65	
	Hardness	0.0578	2.20	
	Nitrate	-0.401	1.42	
Chicago Ship Canal, Illinois, Sta. 4	TDS	-0.0983	0.661	
	TOC	-0.0297	0.985	
	SS	0.151	1.46	
	Hardness	-0.0858	0.874	
	Nitrate	0.576	-0.017	
Illinois River, Illinois, Sta. 5	TDS	0.032	14.9	
	TOC	-0.159	1.91	
	SS	-0.530	1.94	
	Hardness	-0.0364	1.03	
	Nitrate	-0.272	14.9	
Vermillion River, Illinois, Sta. 6	TDS	0.211	1.61	
	TOC	0.208	0.0401	
	SS	-1.18	1.67	
	Hardness	0.170	1.53	
	Nitrate	-1.06	0.904	

(continued)

APPENDIX (continued)

Location	Water Quality Constituent log (mg/ℓ)	$y_t = A \cos (wt + C) + mt$ A	C	m
Eureka Lake, Illinois, Sta. 7	TDS	0.180	2.17	
	TOC	0.0597	34.41	
	SS	-0.553	2.15	
	Hardness	0.156	1.79	
	Nitrate	-0.413	2.09	
Canton Lake, Illinois, Sta. 8	TDS	0.134	-3.43	
	TOC	-0.133	2.00	
	SS	-0.742	1.93	
	Hardness	-0.157	-6.61	
	Nitrate	-0.733	0.385	
Sangamon River, Illinois, Sta. 9	TDS	0.0806	1.71	
	TOC	-0.0846	1.49	
	SS	-0.979	1.40	
	Hardness	0.0753	1.46	
	Nitrate	-2.019	1.22	